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INTRODUCTION TO QUANTUM INFORMATION/COMPUTING

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13. ABSTRACT (Maximum 200 Words) Quantum Information Technology (QIT) is a relatively new area of research whose purpose is to take advantage of the quantum nature of matter and energy to design and build quantum computers which have the potential of improved performance over classical approaches. This report is designed to give the individual, who has little or no knowledge of QIT, an overview of the area by presenting the various disciplines involved in the development. The material is presented in such a way as to familiarize the reader, with a science and engineering background, with the concepts involved to a sufficient depth to provide an overall understanding. This report, in no way, covers all that is happening in this field of research. The information in this report has been extracted from a variety of sources that are enumerated in the List of References. The subject matter includes an introduction to quantum mechanics and associated mathematics, examples of simple quantum systems, information theory, and examples of some quantum algorithms and simple physical implementation of quantum systems for application to QIT.				
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1.0 Introduction

1.1 Classical versus Quantum Computing

Present day computer technology is based on classical physics as the model for the devices which are used to implement the familiar Von Neumann architecture. Although the design of these devices depends on the application of quantum mechanics to the design process and for our understanding of why and how they work, performing a computation, storing the results and making actual measurements is strictly a classical exercise. We move charges around to process data and store the results in domains consisting of charge which is a classical parameter. In some cases we use magnetic fields (tape) storing bits of information as small regions of magnetization. These are just some examples of classical parameters used in classical computing. Underlying all of this is the quantum nature of the processes themselves which are hidden because what we actually measure classically is averages of quantum processes and any features that identify the quantum nature are averaged out. The quantum world is very chaotic and, in general, exhibits very little coherence. If we could in some way maintain sufficient coherence for a long enough period of time to perform a computation we could use the quantum nature of matter as the basis for a computational “paradigm”.

The fundamental unit of classical information as defined by Shannon is the binary digit or what we call a bit of information¹. It is a scalar quantity – it has a value or “state” of 0 or 1 which may be implemented physically as the absence or presence of charge. The capacity of classical communication channels is defined in terms of the number of bits of information. The capacity of an information storage system is defined by the number of bits of information that can be stored. The fundamental unit of information in quantum information is the quantum bit or qubit². A qubit is a vector quantity which suggests that it may represent more “information” than a bit. A qubit may have a value or “state” of 0 or 1 or any superposition, thereof. As an example, an electron, a simple quantum mechanical system, has an intrinsic spin (physically represented by a “spin angular momentum” vector) which is strictly a quantum mechanical concept that has no classical definition. An electron may be in a spin state of 0 (i.e. spin up) or a spin state of 1 (i.e. spin down) or a linear superposition of both. We define these two states $|\text{spinup}\rangle$ and $|\text{spindown}\rangle$ as the bases (since they are orthogonal) of a two dimensional representation of the spin of an electron.

$$|\text{spinstate}\rangle = a|\text{spinup}\rangle + b|\text{spindown}\rangle$$

Figure 1.1 shows a geometric representation of a qubit as a vector ($|\Psi\rangle$) on what is referred to as the Bloch Sphere. One can represent this qubit as

$$|\Psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$

The Dirac Bra-Ket notation for a vector $|\ \rangle$ will be discussed more in Chapter 2.

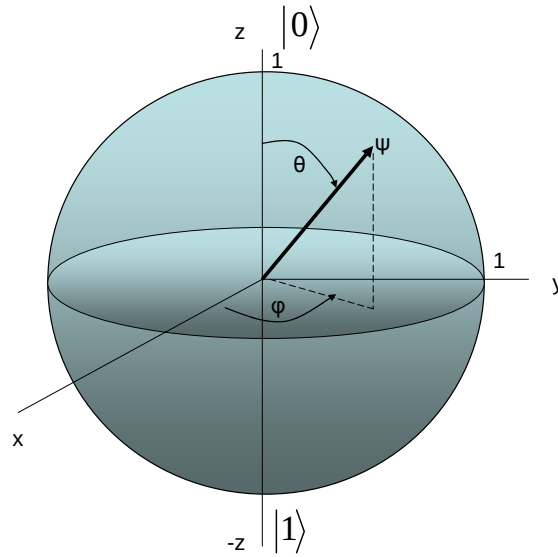


Figure 1.1 Bloch Sphere

The qubit, in this case, is in neither of the two basis states but is in a superposition of both. A classical bit can only take one the two states in the respective z and $-z$ direction. We will see later on in Chapter 4, how this affects the information associated with this quantum state and compare it against the information of a classical bit as defined by Shannon.

1.2 The Wavelike Nature of Material Particles

It was deBroglie who first suggested that particles exhibit a wavelike nature and leading to a formulation of quantum mechanics which was not based on classical Newtonian mechanics³. The idea that particles exhibited a wavelike nature was experimentally verified by observation of electron diffraction and interference. It was a well know fact that electromagnetic waves (i.e.optical) formed an interference pattern after illuminating a double slit. This pattern was a result of both diffraction and interference of the light at and beyond the slits. DeBroglie defined the wavelength of the particle as $\lambda = h / p$ where λ is the wavelength, h is Planck's constant, and p is the linear momentum of the particle. Figure 1.2 shows the double slit experiment for both photons and material particles. Notice that the wavelength of the particle is dependent on the momentum of the particle whereas the photon determines its wavelength from its frequency

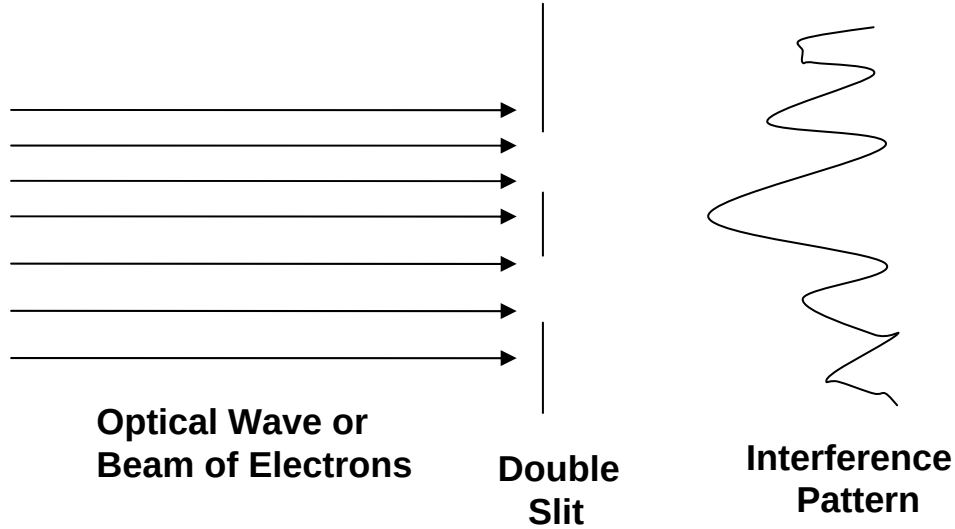


Figure 1.2 Double slit experiment for particles exhibiting a wavelike nature.

The frequency of both photons and material particles is given by $f = E/h$ where f is the frequency, E is the energy, and h is Plank's constant.

and the speed of light or $\lambda_{\text{photon}} = f c$. The velocity of a particle wave is determined by the linear momentum of the particle (linear momentum = mass times linear velocity). In order to keep both the classical mechanical particle theory (the particle is a point object in space) and wave mechanical theory (the particle is a wave with finite extent) consistent with each other, the wave packet or group velocity must be equal to the velocity of the classical particle or particles. The above definition of a quantum particle led to the formulation that one can define the free particle in the x direction at time t as a wavefunction of the form

$$\Psi(x, t) = \sin 2\pi(\nu t - \frac{x}{\lambda}) = \sin \frac{2\pi}{h}(Et - px)$$

where ν = frequency

λ = wavelength

E = total energy of the particle.

p = momentum

h = Planck's constant = $6.6260755 \times 10^{-34}$ Joule-seconds

As a result of this definition, one can use the standard classical wave equation to formulate a differential equation for the behavior of particle waves much like Maxwell did for electromagnetic fields. The equation is given as

$$\frac{\partial^2}{\partial x^2} \Psi(x,t) - \frac{1}{u^2} \frac{\partial^2}{\partial t^2} \Psi(x,t) = 0$$

It can be shown that the phase velocity u may be defined as

$$u = \frac{h\nu}{\sqrt{2m(E - V(x))}}$$

resulting in the time independent one dimensional Schrodinger Wave Equation for a particle of mass m with total energy E in a potential of $V(x)$ and is given by

$$\frac{\partial^2}{\partial x^2} \Psi(x,t) - \frac{2m[E - V(x)]}{h^2} \Psi(x,t) = 0$$

where $V(x)$ = potential energy at point x due to some type of potential field, usually electrostatic.

More will be said about this in Chapter 3.

1.3. Purpose and Outline of Report

Quantum Information Technology (QIT) is relatively new area of research whose purpose is to take advantage of the quantum nature of matter and energy to design and build quantum computers which have the potential of improved performance over classical approaches. This report is designed to give the individual, who has little or no knowledge of QIT, an overview of the area by presenting the various disciplines involved in the development. The material is presented in such a way as to familiarize the reader with a science and engineering background with the concepts involved to a sufficient depth to provide an overall understanding. This report in no way covers all that is happening in this field of research. The information in this report has been extracted from a variety of sources that are enumerated in the List of References. It is suggested that the ambitious reader consult these excellent references for a more in depth understanding of the subject matter especially references 2,3,5,10 and 21.

Chapter 2, Review of Mathematical Concepts lays down the foundation for understanding the chapters that follow. Most of the mathematics should be familiar to most individuals involved in science and engineering and serves only as a refresher. Any mathematical equations presented in following chapters are included not to provide complete mathematical justification (it is not intended to distract the reader by flooding them with a complete mathematical development) but only to present to the reader an understanding of the functions, operators, parameters, and relationships involved in the many concepts and processes being discussed. Like a picture, an equation is worth a thousand words! The chapter starts out with a quick review of vector analysis, and Hilbert spaces with definitions of basis, dimension, and coordinates⁴. This is followed by the concept of functions as vectors and the mathematics of linear operators acting on these functions⁵. The Dirac notation for this mathematics is presented and addresses the dual space of linear functionals and operators. The Dirac notation is used throughout quantum mechanics and quantum information and the reader should become familiar with this powerful representation. How vectors and operators may be represented lays the foundation for the matrix approach to Quantum Mechanics or what is referred to as Matrix Mechanics. A review of the eigenvalue equation is presented since it is the basis for solving for

the steady state solutions of quantum mechanical systems. Finally the concept of the tensor product of state spaces is discussed to acquaint the reader with the representation of several isolated (or even interacting) composite physical systems using one basis representation. It is recommended that the reader not dwell too long on this chapter. For a first reading it is sufficient to get a familiarity with the concepts. However, the reader should leave this chapter at least with an understanding of the Dirac notation which is used throughout the report and in the quantum literature and with an understanding of what is meant by commuting observables.

Chapter 3, Review of Quantum Mechanics, begins with a very brief introduction to the classical Hamiltonian⁶ (or total energy of a system) and then presents the postulates of Quantum Mechanics. The use of the density operator in specifying the state of a quantum system is presented along with the meaning of pure state and statistical mixture of states. What is meant by projection operators and observables and commutation rules which are the basis for the uncertainty principle are discussed along with the Positive Operator-Valued Measure (POVM) which is useful when one wants to get some insight into the statistics of a measurement. Quantum interference is demonstrated and its relationship to quantum entanglement is shown. The chapter wraps up with a presentation of angular momentum and spin (an important concept in Spintronics). There is a very brief discussion on the interaction of electromagnetic (EM) fields with atoms via the concept of the quantized EM field represented by photons. The contents of chapters 2 and 3 are summarization of the same topics in reference 5. The notation was kept the same so that the reader could easily go from this report to reference 3 without a redefinition of variables, operators, and equations.

Chapter 4, Information Theory, starts out with a brief review of Shannon's Classical Information Theory with concepts like mutual and self information and entropy. Several distance measures are presented. This is followed by quantum information and the Von Neumann Entropy as a measure of quantum information and the distance measures such as fidelity and trace distance between quantum states. Finally, the concept of a qubit is presented along with some examples and a comparison between the classical Shannon Entropy and Von Neumann Entropy.

Chapter 5. Simple Quantum Mechanical Systems, provides an understanding of several simple quantum systems which can be useful in understanding QIT device development. Although the systems presented, in general, may not be useful for practical applications they will hopefully provide an insight to the reader for his understanding of those systems presently being looked at by the QIT research community. The chapter starts out with the simplest of all, the free particle which highlights the wave nature of matter. The particle is then placed in a potential well and then in the vicinity of a potential barrier. The possible states of the particle under both these conditions is presented. Finally, we show the possible states for a one dimensional quantum harmonic oscillator. This is derivable from the classical harmonic oscillator which may be implemented by a weight hanging on a coiled spring with spring constant k .

Chapter 6, presents some physical implementations of quantum systems. It starts out with the Penning Trap⁷ (geonium atom). The Penning Trap is a device which permits the trapping of an electron or swarms of electrons in a confined space for the purpose of creating various quantum states that may be used for QIT. The trapping and control of the states is accomplished through use of a vector potential and a quadrupole electrostatic potential. Some of the research presently being conducted is based on variations of this Penning Trap. How one implements quantum dots, quantum wells, and quantum wires give a beginning insight on how one might build a solid state quantum computer and transmit quantum state information.

Chapter 7, Quantum Algorithms presents two separate examples on the increased performance of a quantum approach over a classical approach to computing². The first is the

search algorithm developed by Grover. This section presents the algorithm and how it can be applied to a 4 bit/pixel image as a specific example. This is followed by Super Dense coding which demonstrates how one can communicate more information using a qubit rather than using a classical bit.

There is a brief summary chapter that pulls everything together so that the reader may see the impact of the forest without being distracted by the trees. It might be useful for the reader to first read this last chapter to get a quick overview before beginning to read this report from the beginning.

The Glossary at the end is a list of many terms used in the literature that may be useful if the reader decides to pursue this subject further.

2.0 Review of Mathematical Concepts

2.1 Vectors.

A vector can be defined in the most general sense as a quantity that has both magnitude and direction where the direction is determined within some reference frame and the magnitude is the value of the quantity. The most common reference frames are those that are geometrically depicted as a set of axes at right angles to each other. However, this geometrical representation is usually necessary only for visualization of the space and is not necessary to perform mathematical operations on vector spaces. A vector may also be defined on a field of scalars K , either real or complex, which have some relationship to each other resulting from some measurement such as the height, weight, and age of a person. In this case we have defined the components of the vector and do not have any indication of its direction or magnitude although operations may be made on this vector to obtain magnitude and direction once we have defined a vector space and basis in which to perform these operations.

2.2 Vector Spaces.

A vector space V is the set of all vectors on which rules of addition and scalar multiplication have been defined. For the vectors u and v to be considered a part of a vector space, $u+v=w$, and $ku=w_1$ where $u, v, w, w_1 \in V$, $k \in K$ where $\in$ denotes “is a member of”. In addition to these basic rules there are several other axioms which define a vector space V over the field of scalars K . These axioms identify the zero vector, the meaning of a negative vector, commutative rules, etc.

2.3 Hilbert Space.

This is a vector space in which there is a scalar product defined and a norm is defined on this scalar product. The scalar product of two vectors is defined as $|u| |v| \cos \theta$ where $| \cdot |$ denotes magnitude and θ is the angle between the directions of the two vectors. Likewise, the norm of a vector is defined $\sqrt{|u|^2}$ which is the square root of the scalar product of the vector with itself and represents the magnitude of the vector. Another feature of Hilbert Space is that it is defined on a field of scalars that are complex numbers and that the space is considered to be “complete”. Completeness will be of little concern for this report since it becomes useful only if we wish to present proofs of theorems about vectors in Hilbert Space.

2.4 Basis and Dimension.

A vector space V is said to be n -dimensional if there exists linearly independent vectors $e_1, e_2, \dots, e_n$ which span V . The sequence $(e_1, e_2, \dots, e_n)$ is then called the basis of V . The set of vectors are linearly dependent if there exist scalars $a_1, a_2, \dots, a_n \in K$ not all of them zero, such that

$$a_1 e_1 + a_2 e_2 + \dots + a_n e_n = 0$$

This relationship always holds if the a 's are all zero. If it holds only in the case where all a 's are equal to zero, then the vectors are said to be linearly independent.

2.5 Coordinates.

Let $\{e_1, \dots, e_n\}$ be the basis of an n -dimensional vector space V over a field K , and let v be any vector in V . The basis of the space is said to generate the space in the sense that any vector in the space is a linear combination of the e_i . That is

$$v = a_1 e_1 + a_2 e_2 + \dots + a_n e_n$$

in this case the particular scalars a_i are called the coordinates of the vector v in this basis

representation and the n -tuple $(a_1, \dots, a_n)$ is the coordinate vector of v relative to the basis $\{e_i\}$.

2.6 Functions as vectors.

In wave mechanics, which is the basis for the theory on quantum mechanics, the central object is the wavefunction of a quantum mechanical system which represents the state of the system at any time t . We will first look at the set of continuous functions that are square integrable (called the set L^2) and have a structure in Hilbert Space, i.e.,

$$\int d^3r |\Psi(\mathbf{r}, t)|^2 = 1$$

where we have set the value of the integral to 1 so that it represents a probability although it may have any value less than infinity. Here $\mathbf{r}$ refers to the usual spatial coordinates which may be represented as rectangular, spherical, cylindrical, etc. The coordinates best suited for representation will depend mainly on the geometry of the system. Another condition is that the functions are everywhere defined, continuous, and infinitely differentiable. This additional restriction is then a subspace of L^2 called the set F and represents a set of “sufficiently regular” functions. Unless otherwise specified, all further development will omit the time dependence. This will be addressed when we present the Schrodinger Wave equation.

2.7 Wave Function Space F .

2.7.1. The Scalar Product and Norm.

It can easily be shown that F satisfies the requirements of a vector space. As a result we can define the scalar product of two vector elements $\Phi(\mathbf{r})$ and $\Psi(\mathbf{r})$ as

$$(\Psi, \Phi) = \int d^3r \Phi^*(\mathbf{r}) \Psi(\mathbf{r})$$

(* denotes complex conjugation) which is the scalar product of $\Psi(\mathbf{r})$ by $\Phi(\mathbf{r})$ and which always converges if the vectors belong to F . If the above integral is zero, we say that the vectors are orthogonal. The scalar product of a vector with itself is given as

$$(\Psi, \Psi) = \int d^3r \Psi(\mathbf{r})^* \Psi(\mathbf{r})$$

and its square root is the norm of the vector.

2.7.2. Linear Operators.

A linear operator A is defined by a mathematical entity which associates with every function $\Psi(\mathbf{r}) \in F$ another function $\Psi'(\mathbf{r})$, with the correspondence being linear:

$$\begin{aligned}\Psi'(\mathbf{r}) &= A \Psi(\mathbf{r}) \\ A[\lambda_1 \Psi_1(\mathbf{r}) + \lambda_2 \Psi_2(\mathbf{r})] &= \lambda_1 A \Psi_1(\mathbf{r}) + \lambda_2 A \Psi_2(\mathbf{r})\end{aligned}$$

2.7.3. Product of Operators.

Let A and B be two linear operators. Their product AB is defined by

$$(AB) \Psi(\mathbf{r}) = A[B\Psi(\mathbf{r})]$$

with B acting first followed by A . In general $AB \neq BA$. We define the commutator of A and B as

$$[A, B] = AB - BA$$

This concept is an important concept in Quantum Mechanics and will be further applied later in this report.

2.8 Discrete Orthonormal Bases in F .

2.8.1 Definition.

Let us consider a set of functions in F with discrete indices i ($i = 1, 2, \dots, n$):

$$u_1(\mathbf{r}) \in F, u_2(\mathbf{r}) \in F, \dots, u_i(\mathbf{r}) \in F, \dots$$

The set is orthonormal if

$$(u_i, u_j) = \int d^3r u_i(\mathbf{r})^* u_j(\mathbf{r}) = \delta_{ij}$$

(where δ_{ij} is the kronecker delta function) and it constitutes a basis if every function in F can be expanded in one and only one way such that

$$\Psi(\mathbf{r}) = \sum_i c_i u_i(\mathbf{r})$$

2.8.2. Components of a Wave Function in $\{u_i(\mathbf{r})\}$.

To find the components of a wave function in the above basis one need only to compute the scalar product of the basis with the wave function such as

$$c_i = (u_i, \Psi) = \int d^3r u_i(\mathbf{r})^* \Psi(\mathbf{r})$$

The set of coordinates c_i represent the wavefunction in the $\{u_i(\mathbf{r})\}$ basis. That is, knowing the coordinates is equivalent to knowing the wavefunction as long as the basis is specified.

2.8.3. Scalar Product in Terms of the Components.

It can be shown that

$$(\Phi, \Psi) = \sum_i b_i^* c_i \quad \text{where the } b_i \text{ are coordinates of } \Phi$$

$$\text{and} \quad (\Psi, \Psi) = \sum_i |c_i|^2 \quad \text{which is the square of the norm}$$

2.8.4. Bases not Belonging to F.

Up to now we have discussed discrete bases in F for the representations of wavefunctions. There are two more types of bases that are important when discussing continuous systems using spatial coordinates. These are represented by plane waves and continuous Dirac delta functions. These functions are not square integrable and therefore are not in F. In general, a QM wavefunction in space can be represented as a superposition of plane waves similar to what is done in classical electromagnetic theory where there is a fourier transform relationship between the wave in space and its representation in the frequency domain. In the QM case, however, the wavevector (which is related to the frequency of the plane wave) is represented by the momentum of the particle. We can write the wavefunctions (in one dimension) in both these domains as

$$\Psi(x) = \int_{-\infty}^{\infty} dp \bar{\Psi}(p) v_p(x)$$

$$\bar{\Psi}(p) = (v_p, \Psi) = \int_{-\infty}^{\infty} dx v_p^*(x) \Psi(x)$$

where $v_p(x) = 1/\sqrt{2\pi\hbar} e^{ipx/\hbar}$ and $\hbar$ is Planck's constant h divided by 2π .

The function $\bar{\Psi}(p)$ now fulfills a role of a wavefunction with a continuous index p rather than the discrete index i in defining the coordinates of the wavevector. Many quantum systems may be represented by both a continuous and discrete set of bases.

Another basis can be represented by a set of delta functions such that

$$\xi_{\mathbf{r}_0} = \delta(\mathbf{r} - \mathbf{r}_0)$$

and represents a set of delta functions at the points $\mathbf{r}_0$. These functions are not square-integrable and therefore are not part of F. However, we can write our wavefunctions using the above basis which will create a set of wavefunctions which are members of F such that

$$\Psi(\mathbf{r}) = \int d^3r_0 \Psi(\mathbf{r}_0) \xi_{\mathbf{r}_0}$$

$$\Psi(\mathbf{r}_0) = (\xi_{\mathbf{r}_0}, \Psi) = \int d^3r \xi_{\mathbf{r}_0}(\mathbf{r}) \Psi(\mathbf{r})$$

The first equation allows one to write the wavefunction in the delta function basis while the second integral gives the coordinate at a point $\mathbf{r}_0$ by taking the scalar product of a specific delta function basis element with the wavefunction.

One can generalize this for any set of bases w_α which are continuous and orthonormal and labelled by a continuous index α and that satisfy the orthonormality and closure relations such that

$$(w_\alpha, w_{\alpha'}) = \int d^3r w_\alpha^*(\mathbf{r}) w_{\alpha'}(\mathbf{r}) = \delta(\alpha - \alpha') \quad \text{orthonormalization}$$

$$\int d\alpha w_\alpha(\mathbf{r}) w_\alpha^*(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad \text{closure}$$

To find the components $c(\alpha)$, one merely needs to compute the scalar product of $w_\alpha(\mathbf{r})$ with the wavefunction $\Psi(\mathbf{r})$. Also, as in the other examples above it can be shown that the scalar product of the wavefunctions $\Psi(\mathbf{r})$ and $\Phi(\mathbf{r})$ is merely

$$(\Phi, \Psi) = \int d\alpha b^*(\alpha) c(\alpha)$$

where the $b(\alpha)$ and $c(\alpha)$ are the coordinate representations for the two wavefunctions.

2.9 The Dirac Notation

In the above presentations we have shown some of the various ways that wavefunctions may be expressed and evaluated using the familiar Calculus. Also one may represent the state of the system by a geometrical vector which need not be referred to any set of coordinates (basis). The Dirac notation allows us to represent the state of a system and any of the operations on that state to be expressed in this very easy to use symbolic representation. The space in which the state resides is called the state space and is represented by ε . A vector in ε is called a ket vector and represented by the symbol $|\rangle$. What one places within the symbol depends on what the representation of the particle state may be. For example if the ket is representing a wavefunction then one would write $|\Psi\rangle$ or if one were representing a spin $\frac{1}{2}$ particle one would write $|1/2\rangle$. As is evident, the notation is very powerful and may be used to describe any state of a system be it discrete or continuous. When we talk about the space of all square integrable functions, the vector space for kets is represented by ε_r which is the state space of a spinless particle, i.e., it is represented only by an element in F . Therefore if $\Psi(\mathbf{r}) \in F$ then $|\Psi\rangle \in \varepsilon_r$. This space has its familiar components in x, y, z , i.e., $\varepsilon_x, \varepsilon_y, \varepsilon_z$. At this point we are representing a vector by its components in a specific coordinate system which may be considered on same level as all other coordinate systems. The power and simplicity of this notation lies in the fact that we can use it to define a representation for the state of systems and define a “linear algebra” by merely how we juxtapose the symbols. This will be shown next.

2.9.1. Linear Functionals/Scalar Product

First we may represent the scalar product of the pair of kets $|\Phi\rangle$ and $|\Psi\rangle$ by $(|\Phi\rangle, |\Psi\rangle)$ with its usual association with a complex number. This is one way to represent the scalar product, but the more powerful way in the Dirac notation is $\langle\Phi|\Psi\rangle$ where $\langle\Phi|$ is called a bra vector. We now have what is usually referred to as the Dirac Bra-Ket notation which is taken from the word “bracket”. To define the bra vector, we need to define a dual space for the ket vectors which is a space of linear **functionals** which assign a complex number to each ket. Note that a **linear operator** assigns a ket to a ket. For each ket we may define a bra which performs the operation of a linear functional. When the scalar product is taken between a bra and a ket we define a linear functional operation which results in a complex number. For example,

$$\langle\Phi|\Psi\rangle = (|\Phi\rangle, |\Psi\rangle) \text{ which is a complex number}$$

Every ket has associated with it a bra in the space ε^* . This association is shown by

$$\langle\lambda\Psi| \leftrightarrow |\lambda\Psi\rangle$$

2.9.2. Linear Operators

A linear operator A associates with every ket $|\Psi\rangle$ another ket $|\Psi'\rangle$ with a linear correspondence such that

$$|\Psi'\rangle = A |\Psi\rangle$$

We define the product of two operators A and B as AB such that

$$(AB) |\Psi\rangle = A(B|\Psi\rangle)$$

The commutator of A and B , where AB is not necessarily equal to BA , is defined as

$$[A, B] = AB - BA$$

If $AB=BA$ we say that the operators commute. Commuting operators are an important concept in QM as we shall see later.

Finally, we call the matrix elements of A between $|\Phi\rangle$ and $|\Psi\rangle$, the scalar product of $|\Phi\rangle$ with the ket $A |\Psi\rangle$

$$\langle\Phi|A|\Psi\rangle$$

We will say more about this later when we talk about matrix representations of kets and operators.

2.9.3. Projection operators

Let us now arrange the kets and bras in a manner where $|\Psi\rangle\langle\Phi|$ represents an operator. To see this, let us operate on some ket $|X\rangle$ with the above operator. We get

$$|\Psi\rangle\langle\Phi||X\rangle.$$

It is customary to eliminate one vertical bar when we juxtapose so that we can write

$$|\Psi\rangle\langle\Phi|\Psi\rangle$$

By the previously shown notation for a scalar product, we can see that $\langle\Phi|\Psi\rangle$ is merely a complex number and the resultant operation results in a ket. The order in which we write the kets and bras determines their function and what they represent.

We can define an operator $P_\Psi = |\Psi\rangle\langle\Psi|$ where here the ket $|\Psi\rangle$ is normalized such that $\langle\Psi|\Psi\rangle = 1$ and apply this to an arbitrary ket $|\Phi\rangle$ we see that

$$P_\Psi|\Phi\rangle = |\Psi\rangle\langle\Psi|\Phi\rangle$$

we again have a ket multiplied by a complex number. We can see that this operator's function is to orthogonally project ket $|\Phi\rangle$ onto the ket $|\Psi\rangle$. Since this is a projection operator, $P_\Psi = P_\Psi^2$. Multiple projections give the same results as a single projection.

2.9.4. Adjoint Operators/Hermitian Conjugation

So far we have shown the action of an operator on the kets. We have also shown that there is a one to one correspondence between the kets and bras (this may not be always necessarily true, but for our purposes will suffice). The bra associated with each ket is a linear functional which permits us to perform scalar product operations between the space $\mathcal{E}$ (the space of kets) and its associated dual space $\mathcal{E}^*$ (the space of bras). In a similar manner, we can associate with every operator A acting on a ket, a corresponding operator $A^\dagger$, called the adjoint of A , acting on a bra. Some comments which help to define the operator are:

1. Defining the action of the operator $A^\dagger$ on the bras we can say that the operator $A^\dagger$ associates with the bra $\langle\Psi|$ corresponding to the ket $|\Psi\rangle$ the following relationships

$$|\Psi'\rangle = A|\Psi\rangle \leftrightarrow \langle\Psi'| = \langle\Psi|A^\dagger.$$

or for all Φ and Ψ we can write

$$\langle\Psi|A^\dagger|\Phi\rangle = \langle\Phi|A|\Psi\rangle^*$$

Relationships between an operator and its adjoint are given by

$$\begin{aligned}(A^\dagger)^\dagger &= A \\ (\lambda A)^\dagger &= \lambda^* A^\dagger \\ (A + B)^\dagger &= A^\dagger + B^\dagger \\ (AB)^\dagger &= B^\dagger A^\dagger\end{aligned}$$

A simple set of rules to follow in performing Hermitian Conjugation are

To obtain the Hermitian conjugate (or the adjoint) of any expression composed of constants, kets, bras, and operators, one must:

Replace – the constants by their complex conjugates
the kets by the bras associated with them
the bras by the kets associated with them
the operators by their adjoints

Reverse the order of the factors (the position of the constants is of no importance)

Finally, an operator A is said to be Hermitian if $A = A^\dagger$.

2.10. Representations in State Space

2.10.1 Representing kets, bras, and operators

So far we have just talked about the general notation used for vectors and operators without any reference to specific representation. We must be able to express these elements in some form that make computation possible. We will now present in summary form how this is accomplished.

To represent a ket/bra in the $\{|u_i\rangle\}$ basis we need only represent coordinates of the ket/bra in this basis or the set of numbers $c_i = \langle u_i | \Psi \rangle$ and arrange them in a column vector and for a bra Φ we arrange the components in a row vector as follows:

$$\begin{array}{ccc} \left(\begin{array}{c} \langle u_1 | \Psi \rangle \\ \langle u_2 | \Psi \rangle \\ \vdots \\ \langle u_i | \Psi \rangle \\ \vdots \end{array} \right) & & (\langle \Phi | u_1 \rangle \quad \langle \Phi | u_2 \rangle \quad \dots \quad \langle \Phi | u_i \rangle \quad \dots) \\ \text{Ket} & & \text{Bra} \end{array}$$

If one then multiplies the above two matrices (Bra times Ket), one gets a single number which is the scalar product $\langle \Phi | \Psi \rangle$. A similar representation can be shown for the continuous basis $\{|w_\alpha\rangle\}$ discussed in previous sections. This example is shown below.

$$\downarrow \begin{pmatrix} \vdots \\ \langle w_\alpha | \Psi \rangle \\ \vdots \end{pmatrix}$$

Ket representation in a continuous basis

Here we have a matrix with continuous indices α increasing in the direction of the arrow as opposed to the discrete indices in the previous examples. We can draw a similar matrix for the bra as a row vector.

In order to represent an operator in the same basis as above, we use a square matrix. The elements of this matrix operator in this basis are given by

$$A_{ij} = \langle u_i | A | u_j \rangle \text{ for the discrete case}$$

$$\text{and} \quad A(\alpha, \alpha') = \langle w_\alpha | A | w_{\alpha'} \rangle \text{ for the continuous case}$$

with resulting matrices

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1j} & \dots \\ A_{21} & A_{22} & \dots & A_{2j} & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{i1} & A_{i2} & \dots & A_{ij} & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

for discrete case

$$\begin{matrix} & \xrightarrow{\alpha'} \\ \alpha \downarrow & \begin{pmatrix} \vdots \\ \dots & \dots & A(\alpha, \alpha') \end{pmatrix} \end{matrix}$$

for continuous case

The matrix representation for the adjoint operator $A^\dagger$ is derived from A by interchanging rows and columns and taking the complex conjugate. If A is Hermitian then it can be shown that its diagonal elements are real numbers.

We may not always want to work in a particular basis so we need to define a procedure to transform operators, kets, and bras in a new basis. To do this we define a transformation matrix $S_{ik} = \langle u_i | t_k \rangle$ where the u_i are the old basis and the t_k are the new basis. To obtain a ket, bra, or operator in the new basis from its components in the old basis we use

$$\langle t_k | \Psi \rangle = \sum_i S_{ki}^\dagger \langle u_i | \Psi \rangle \quad \text{for a ket}$$

$$\langle \Psi | t_k \rangle = \sum_k S_{ik} \langle t_k | \Psi \rangle \quad \text{for a bra}$$

$$A_{kl} = \sum_{i,j} S_{ki}^\dagger A_{ij} S_{jl} \quad \text{for operator from new to old coordinates}$$

$$A_{ij} = \sum_{k,l} S_{ik} A_{kl} S_{lj}^\dagger \quad \text{for operator from old to new coordinates}$$

2.10.2. Eigenvalue Equations

The eigenvalue equation is given by

$$A |\Psi\rangle = \lambda |\Psi\rangle$$

where $|\Psi\rangle$ is an eigenvector of the operator A and λ is the eigenvalue. The eigenvectors of an operator are those vectors which, upon operation by A , change only in their length. This equation only possesses certain solutions when λ takes on certain values. These eigenvalues are referred to as the spectrum of the operator A . It is customary to specify all the eigenvectors as being normalized in order to avoid certain problems not to be covered here. When there is only one eigenvector for each eigenvalue, then we say that the eigenvalue is non-degenerate. If the eigenvalue has g eigenvectors associated with it, then we say the eigenvalue is g -fold degenerate and is associated with a g -dimensional eigensubspace within the space that the operator is acting. Degeneracy adds another level of complexity to the problem and will not be addressed to any great extent at this point. Where necessary it will be addressed to clarify some examples of physically degenerate systems such as those exhibiting angular momentum.

In order to compute the eigenvalues and eigenvectors of an operator one needs to first represent the operator in some basis and then compute the matrix form $[A]$ of the operator as was done above. The eigenvalues are then the roots of what is called the characteristic equation of the operator which essentially boils down to solving for the N values of λ as follows:

$$\begin{bmatrix} A_{11} - \lambda & A_{12} & A_{13} & \dots & A_{1N} \\ A_{21} & A_{22} - \lambda & A_{23} & \dots & A_{2N} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ \vdots & \vdots & \vdots & \dots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \dots & A_{NN} - \lambda \end{bmatrix} = 0$$

Computing the eigenvectors is accomplished by substituting back into the above eigenvalue equation and solving for the eigenvectors. However, this procedure can be found in most texts on linear algebra⁴.

Finally, the eigenvectors of the operator A belonging to two different eigenvalues are orthogonal and can therefore form a basis upon normalization. Note that this will usually be a basis different than the original representation of the operator A in the characteristic equation. Although the eigenvectors are orthogonal, they may be represented by a linear superposition of the original basis associated with the operator A .

2.10.3. Observables

A Hermitian operator A is an observable if its eigenvectors form a basis in the space $\mathcal{E}$. In the most general sense for a mixed system of discrete and continuous wavefunctions must follow the closure relation (we are assuming that the continuous part is non-degenerate)

$$\sum_n \sum_{i=1}^{g_n} |\Psi_n^i\rangle\langle\Psi_n^i| + \int_{\nu_1}^{\nu_2} d\nu |\Psi_\nu\rangle\langle\Psi_\nu| = \mathbf{1} \quad (\text{the identity operator})$$

where the $|\Psi_n^i\rangle$ are the basis for the discrete spectrum of n eigenvalues and g_n is the degeneracy of the i_{th} eigenvalue for a spectrum of n eigenvalues. The $|\Psi_\nu\rangle$ are the basis for the continuous spectrum where the ν are the continuous index.

2.10.4. Commuting Observables

Here we will present several theorems relating to commuting observables.

Theorem 1. If two operators A and B commute, and if $|\Psi\rangle$ is an eigenvector of A , $B|\Psi\rangle$ is also an eigenvector of A , with the same eigenvalue.

This can be seen by the following expression

$$A(B|\Psi\rangle) = a(B|\Psi\rangle)$$

In QM, an operation on a state is a measurement on that state, so that when we make the measurement B the result is b (the eigenvalue of B) but the state is still an eigenstate of A so that when we follow this by a measurement of A the result will be a (the eigenvalue of A). Also measurements of A can be made independently and without influencing measurements of B to arbitrary precision, and vice versa. When the operators do not commute this statistical independence no longer holds, a fact that is the basis for the Heisenberg Uncertainty Principle which we will discuss later.

Theorem 2. If two observables A and B commute, one can construct an orthonormal basis of the state space with eigenvectors common to A and B .

An important result of this theorem is that once we find the eigenvectors of an operator and can define other operators that commute, then we need not compute the eigenvectors for the commuting operators. In QM, the total energy of a system is defined by the Hamiltonian operator (H) whose eigenvectors may be found by solving the Schrodinger Wave equation for the Hamiltonian (see Chapter 3). Therefore we will have already determined the eigenvectors for all other operators that commute with H once we have found the solution to the Schrodinger Wave equation. We can establish a complete set of commuting observables that best characterize the system under study. For example, in the lowest order approximation to the hydrogen atom spectra, we can measure total energy (H), angular momentum squared (L^2), the z -component of the angular momentum (L_z), z -component of the intrinsic spin (S_z), and the square

of the intrinsic spin (S^2). For a free spinless particle with mass, we can measure the energy (H) and momentum (P).

A complete set of commuting observables (C.S.C.O.) **A, B, C, ...** have property that all observables commute by pairs and specifying the eigenvalues of all the operators determines a unique common eigenvector. Also the C.S.C.O. have a unique set of orthonormal basis of common eigenvectors (to within a phase factor) for all the operators in the set.

2.10.5. Tensor Product of State Spaces.

In 2.9 above, we briefly introduced the concept of a vector space for kets ε_r and spaces $\varepsilon_x, \varepsilon_y$, and ε_z which are spaces for all square integral functions in F but are disjoint. All these are different spaces but one can construct a relationship between these spaces by using a the tensor product. This has great value when one wishes to represent several isolated (or even interacting) physical systems using one basis. Its greatest application in Quantum Information is being able to represent several quantum bits (qubits) which are implemented by two state systems within one tensor product space. For example, the state of a n-qubit register may be represented by a tensor product of the states of each of the two state systems.

By definition, the vector space ε is the tensor product of ε_1 and ε_2 .

$$\varepsilon = \varepsilon_1 \otimes \varepsilon_2$$

if there is associated with each pair of vectors, $|\phi(1)\rangle$ belonging to ε_1 and $|\chi(2)\rangle$ belonging to ε_2 , a vector of ε denoted by

$$|\phi(1)\rangle \otimes |\chi(2)\rangle = \sum_{i,l} a_i b_l |u_i(1)\rangle \otimes |v_l(2)\rangle$$

where the a_i and b_l are components of $|\phi(1)\rangle$ and $|\chi(2)\rangle$ in ε_1 and ε_2 , respectively, and $|u_i(1)\rangle$ and $|v_l(2)\rangle$ are basis vectors in ε_1 and ε_2 , respectively. This correspondence is linear with respect to multiplication by complex numbers, is distributive with respect to vector addition, and the basis for ε is the set of vectors $|u_i(1)\rangle \otimes |v_l(2)\rangle$. The dimension of this new space is the product of the dimensions of ε_1 and ε_2 .

In general, however, we may write the state of the two systems as a composite vector

$$|\Psi\rangle = \sum_{i,l} c_{i,l} |u_i(1)\rangle \otimes |v_l(2)\rangle$$

Since $c_{i,l}$ is not necessarily always equal to $a_i b_l$, there are vectors in ε that are not tensor products of vectors in ε_1 and ε_2 . We will see later that this phenomena results in what is called the quantum entanglement of particles where the state in ε is not a tensor product state. Finally, if the vectors are represented as matrices, the tensor product is the usual one found in matrix algebra. The tensor product is also called the kronecker product.

One may define operators in the space ε . The action of the tensor product of two operators $A(1)$ and $B(2)$ from ε_1 and ε_2 , respectively, on tensor product vectors is given by

$$[A(1) \otimes B(2)] [|\phi(1)\rangle \otimes |\chi(2)\rangle] = [A(1) |\phi(1)\rangle] \otimes [B(2) |\chi(2)\rangle]$$

One may also extend operators in ε_1 and ε_2 into operators in ε as follows:

$$\begin{aligned}\tilde{A}(1) &= A(1) \otimes \mathbf{1}(2) \\ \tilde{B}(2) &= \mathbf{1}(1) \otimes B(2)\end{aligned}$$

where $\mathbf{1}(1)$ and $\mathbf{1}(2)$ are the identity operators in ε_1 and ε_2 , respectively. We then can apply the following expression

$$A(1) \otimes B(2) = \tilde{A}(1) \tilde{B}(2)$$

and further show that $\tilde{A}(1)$ and $\tilde{B}(2)$ commute in ε . Also, as in the case for vectors, there are operators in ε that are not tensor products of operators in ε_1 and ε_2 .

When we write tensor products we usually use the following conventions which avoids using the tensor product symbol

$$\begin{aligned}|\phi(1)\rangle |\chi(2)\rangle &\text{ which is equivalent to } |\phi(1)\rangle \otimes |\chi(2)\rangle \\ A(1) B(2) &\text{ which is equivalent to } A(1) \otimes B(2) \\ A(1) &\text{ is } \tilde{A}(1) \text{ or } A(1).\end{aligned}$$

The last two present some ambiguity but if there are distinctions made between operators and their component spaces, what is meant should be obvious.

3.0 Review of Classical/Quantum Mechanics

3.1 Classical Mechanics

In classical mechanics, the equations of motion a particle of mass m are functions of the position and velocity of the particle which are functions of time⁶. The representation is usually expressed in the form of generalized coordinates (position) and conjugate momentum of each of the generalized coordinates. To avoid any more generality and complexity, we will use the more familiar coordinates given by the position vector $\mathbf{r}$ with components x , y , and z and the conjugate momenta (also known as the linear momentum) expressed as p_x , p_y , p_z . We can write the equations of several measureable quantities such as

$\mathbf{p} = m \mathbf{v}$	momentum of particle with mass m and velocity $\mathbf{v}$
$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r},t)$	total energy of particle (also called the Hamiltonian) where $V(\mathbf{r},t)$ is the potential energy
$\mathbf{L} = \mathbf{r} \times \mathbf{p}$	angular momentum of particle with respect to origin

3.2. The Postulates of Quantum Mechanics^{3,5}

3.2.1. First Postulate:

At a fixed time t_0 , the state of a physical system is defined by specifying a ket $|\Psi(t_0)\rangle$ belonging to the state space $\mathcal{E}$.

This postulate allows one to represent the initial conditions by a state vector.

3.2.2. Second Postulate:

Every measureable physical quantity A is described by an operator A acting in $\mathcal{E}$. This operator is an observable.

We can see now why we defined certain operators as observables since they correspond back to an actual physical measurement in classical mechanics. The leap from classical mechanics to quantum mechanics is made by expressing all measureable quantities from classical mechanics in terms of operators in quantum mechanics, at least for the Shrodinger model of QM.

Before we proceed further, let us look at some very important physical quantities which are represented as operators (observables) in QM. These are:

Classical Measurement	Quantum Operator
$\mathbf{r}$ (position)	$\mathbf{R}$
$\mathbf{p}$ (linear momentum)	$\mathbf{P}$
H (total Energy)	$\mathbf{H}$
$\mathbf{L}$ (angular momentum)	$\mathbf{L}$

If one looks at the expressions for these physical quantities in 3.1 above, we can see that the total energy and angular momentum may be expressed as functions of position, linear momentum and potential energy.

There are two representations in QM which will allow us to define state vectors and operators which correspond to the position and momentum in classical mechanics. These bases are

$$\xi_{\mathbf{r}0} = \delta(\mathbf{r} - \mathbf{r}_0) = |\mathbf{r}_0\rangle \quad \text{called the } \mathbf{r}\text{-representation}$$

$$\nu_{\mathbf{p}0}(\mathbf{r}) = (2\pi\hbar)^{-3/2} e^{i\mathbf{p}_0 \cdot \mathbf{r}/\hbar} = |\mathbf{p}_0\rangle \quad \text{called the } \mathbf{p}\text{-representation}$$

with component vectors $|x_0\rangle, |y_0\rangle, |z_0\rangle$ and $|p_{x0}\rangle, |p_{y0}\rangle, |p_{z0}\rangle$

We can evaluate the components of $|\Psi\rangle$ at a point $\mathbf{r}_0$ and momentum $\mathbf{p}_0$ by

$$\langle \mathbf{r}_0 | \Psi \rangle = \Psi(\mathbf{r}_0) = \int d^3r \delta(\mathbf{r} - \mathbf{r}_0) \Psi(\mathbf{r})$$

$$\langle \mathbf{p}_0 | \Psi \rangle = \bar{\Psi}(\mathbf{p}_0) = \int d^3r (2\pi\hbar)^{-3/2} e^{-i\mathbf{p}_0 \cdot \mathbf{r}/\hbar}$$

where $\bar{\Psi}(\mathbf{p})$ is the fourier transform of $\bar{\Psi}(\mathbf{r})$. Also see section 2.8.4.

The operators associated with the $\mathbf{r}$ - and $\mathbf{p}$ -representations are expressed as follows:

If we are in the $\mathbf{r}$ -representation, the operator $\mathbf{R}$ is merely $\mathbf{R}$ with its components x, y, z . In this representation the $\mathbf{P}$ operator is expressed as $\mathbf{P} = (\hbar/i) \nabla$ where $\nabla = \mathbf{i} d/dx + \mathbf{j} d/dy + \mathbf{k} d/dz$ and $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are unit vectors in the $\mathbf{r}$ -representation.

If we are in the $\mathbf{p}$ -representation the operator $\mathbf{P}$ is merely $\mathbf{P}$ with its components p_x, p_y, p_z . In this representation the operator $\mathbf{R}$ is expressed as $\mathbf{R} = -(\hbar/i) \nabla \mathbf{p}$ where $\nabla \mathbf{p} = \mathbf{i}_{px} d/dp_x + \mathbf{j}_{py} d/dp_y + \mathbf{k}_{pz} d/dp_z$ and where the $\mathbf{i}_{px}, \mathbf{j}_{py}, \mathbf{k}_{pz}$ are unit vectors in the $\mathbf{p}$ -representation along the component axes of p_x, p_y, p_z .

One of the reasons that these two representations are so important is that other operators may be expressed in terms of the $\mathbf{R}$ and $\mathbf{P}$ operators. For example, to obtain the $\mathbf{H}$ operator mentioned above, we need only substitute in the classical Hamiltonian (total energy) the operators in place of the variables $\mathbf{r}$ and $\mathbf{p}$ so that the Hamiltonian operator becomes

$$\mathbf{H} = \mathbf{P}^2/2m + V(\mathbf{R}, t)$$

What this operator looks like in terms of the operators $\mathbf{R}$ and $\mathbf{P}$ will depend on which representation we use. In the $\mathbf{r}$ -representation, the operator $\mathbf{R}$ is merely the variable $\mathbf{r}$ multiplying the operand and the operator $\mathbf{P}$ is a differential operator acting on the operand as discussed above. In the $\mathbf{p}$ -representation, just the opposite is true. With these definitions we will later see how the *Schrödinger* Wave Equation is formed for a variety of Hamiltonians to get a differential equation whose solutions are the eigenvalues and eigenfunctions of the particular quantum system specified by its Hamiltonian. What we are doing is taking an expression for a measureable in the classical world and using it to write an expression of this measureable quantity in the quantum world (i.e., the *Schrödinger* Wave Equation).

We can represent the $\mathbf{R}$ and $\mathbf{P}$ operators as

$$\mathbf{R} = R_1\mathbf{i} + R_2\mathbf{j} + R_3\mathbf{k} \quad \text{and} \quad \mathbf{P} = P_1\mathbf{i} + P_2\mathbf{j} + P_3\mathbf{k}$$

where $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are unit vectors and the R_i and P_i are components of $\mathbf{R}$ and $\mathbf{P}$ in the direction of the unit vectors.

With a little effort we can get the following result for the commutation relations between the components of these operators as:

$$[R_i, R_j] = 0; \quad [P_i, P_j] = 0; \quad [R_i, P_j] = i\hbar \delta_{ij} \quad i, j = 1, 2, 3$$

The commutation relations between these fundamental dynamical variables are important in that they allow us to easily create similar relationships between other observables such as angular momentum.

3.2.3. Third Postulate:

The only possible result of the measurement of a physical quantity A is one of the eigenvalues of the corresponding observable (operator) A .

A measurement A always gives a real value, since A by definition is Hermitian. If the spectrum of A is discrete, the results that can be obtained by measuring A are quantized.

3.2.4. Fourth Postulate (case of a discrete non-degenerate spectrum):

When the physical quantity A is measured on a system in the normalized state $|\Psi\rangle$, the probability $P(a_n)$ of obtaining the non-degenerate eigenvalue a_n of the corresponding observable A is:

$$P(a_n) = |\langle u_n | \Psi \rangle|^2 \quad \text{where } |u_n\rangle \text{ is the normalized eigenvector of } A$$

associated with the eigenvalue a_n .

Fourth Postulate (case of a degenerate discrete spectrum): When the physical quantity A is measured on a system in the normalized state $|\Psi\rangle$, the probability $P(a_n)$ of obtaining the eigenvalue a_n of the corresponding observable is:

$$P(a_n) = \sum_{i=1}^{g_n} |\langle u_n^i | \Psi \rangle|^2 \quad \text{where } g_n \text{ is the degree of degeneracy of } a_n \text{ and}$$

$\{|u_n^i\rangle\}$ ($i = 1, 2, \dots, g_n$) is an orthonormal set of vectors which forms a basis in the eigensubspace ε_n associated with the eigenvalue a_n of A . It can be shown that a change of the basis in ε_n does not affect $P(a_n)$.

In the case of a continuous spectrum (non-degenerate) we define a probability density $\rho(\alpha)$ as

$$\rho(\alpha) = |\langle v_\alpha | \Psi \rangle|^2 \quad \text{where the } |v_\alpha\rangle \text{ are the continuous eigenfunctions of}$$

the operator and the probability of finding a measurement within the interval α and $\alpha + d\alpha$ is

$$d P(\alpha) = \rho(\alpha) d\alpha$$

3.2.5. Fifth Postulate:

If the measurement of the physical quantity A on the system in the state $|\Psi\rangle$ gives the result a_n , the state of the system immediately after the measurement is the normalized projection, $\frac{P_n|\Psi\rangle}{\sqrt{\langle\Psi|P_n|\Psi\rangle}}$, of $|\Psi\rangle$ onto the eigensubspace associated with a_n .

This postulate states one important aspect of measurement in QM. If a system is in a specific state which is a superposition of several eigenstates just before measurement, the state it is found in upon measurement can only be an eigenstate of the associated eigenvalue measured. This obviously begs several questions which we will not address here, especially when we address the time evolution of a state vector governed by the *Schrödinger* Equation.

3.2.6. Sixth Postulate:

The time evolution of the state vector $|\Psi(t)\rangle$ is governed by the *Schrödinger* equation:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \mathbf{H}(t) |\Psi(t)\rangle$$

where $\mathbf{H}(t)$ is the observable (in this case the Hamiltonian operator of the system) and is obtained from the classical Hamiltonian by substituting the $\mathbf{R}$ and $\mathbf{P}$ operators as follows:

$$\mathbf{H} = \mathbf{P}^2/2m + V(\mathbf{R},t)$$

In the $\mathbf{r}$ -representation this would be

$$\mathbf{P}^2 = \mathbf{P} \cdot \mathbf{P} = (\hbar/i) \nabla \cdot (\hbar/i) \nabla = -\hbar^2 \nabla^2 \quad \text{where} \quad \nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

and $V(\mathbf{R},t)$ becomes $V(\mathbf{r},t)$

For this specific case of a Hamiltonian of a spinless particle with a kinetic energy and in a scalar potential $V(\mathbf{r})$, we get the *Schrödinger* equation

$$\frac{d}{dt} |\Psi(t)\rangle = \hbar \nabla^2 |\Psi(t)\rangle + V(\mathbf{r}) |\Psi(t)\rangle$$

For a potential of zero, this reduces to the familiar form of a free particle with the usual complex exponential solutions. One can find an analogy of this for an electromagnetic wave in free space. Once the particle is subjected to a potential, the potential can perturb the free particle in a variety of ways thus generating a variety of different eigenstates both discrete and continuous. Having this flexibility to play with the potential, and hence the states of the system, is important to

researchers developing quantum devices for use in quantum computing. Some examples of this is quantum dots and ion traps.

In general, the observable $\mathbf{A}$ which represents a classically defined physical quantity A is obtained by replacing $\mathbf{r}$ and $\mathbf{p}$ in the expression for A , by the operators $\mathbf{R}$ and $\mathbf{P}$, respectively. There are, however, certain physical quantities which have no counterpart in classical mechanics for which this rule does not apply. They are handled directly by the corresponding observables. An example of this is the intrinsic spin of a particle.

3.3 Pure State, Statistical Mixture of States, and The Density Operator.

When a system is in a state which is perfectly known (probability =1) we say that it is in a **pure state**. The state vector may be formed by an expansion on an orthonormal basis of the state space.

$$|\Psi(t)\rangle = \sum_n c_n(t) |u_n\rangle$$

where the $|u_n\rangle$ defines an orthonormal basis of the state space and $\sum_n |c_n(t)|^2 = 1$.

The **density operator** is defined as

$$\rho(t) = |\Psi(t)\rangle \langle \Psi(t)|$$

The matrix elements of this operator for the basis $|u_n\rangle$ are given by

$$[\rho(t)]_{n,p} = \langle u_n | \Psi(t) \rangle \langle \Psi(t) | u_p \rangle$$

And working out the scalar products this reduces to

$$[\rho(t)]_{n,p} = c_n^*(t) c_p(t)$$

It can easily be shown that the trace of $[\rho(t)]$

$$\text{Tr} [\rho(t)] = \sum_n \rho_{nn}(t) = \sum_n |c_n(t)|^2 = 1$$

The non-pure case or the case for a statistical mixture of states can be formulated by considering a system with a set of probabilities $p_1, p_2, \dots, p_k$ such that $\sum_k p_k = 1$ which are assigned to the possible states $|\Psi_k\rangle$ which the system can find itself in. The probability of finding an eigenvalue a_n when the system is in state $|\Psi_k\rangle$ is given by

$P_k(a_n) = \langle \Psi_k | P_n | \Psi_k \rangle$ where P_n is the projector onto the eigensubspace associated with a_n . We can define a density operator with respect to the state $|\Psi_k\rangle$ as

$$\rho_k = |\Psi_k\rangle \langle \Psi_k| \quad \text{and define an average density operator as}$$

$$\rho = \sum_k p_k \rho_k \quad \text{which finally allows us to write}$$

$$P(a_n) = \text{Tr}\{ \rho P_n \}$$

This is the probability of measuring eigenvalue a_n when the system is a statistical mixture of k states with probabilities p_k .

3.4. Observables and Their Measurement.

3.4.1. The Mean Value of an Observable.

We shall denote the mean value of the observable $\mathbf{A}$ as $\langle A \rangle$. This is its mean value when the system is in a normalized state $|\Psi\rangle$. If $\mathbf{A}$ has the eigenvectors $|a_n\rangle$ with eigenvalues a_n , then the mean value of the measurement is given as

$$\langle A \rangle = \sum_n a_n \times \text{probability of finding the system in state } n = \langle \Psi | \mathbf{A} | \Psi \rangle$$

This says that if we measured the observable many times while the system is in the state $|\Psi\rangle$, then on the average the measurement would yield $\langle \Psi | \mathbf{A} | \Psi \rangle$. Of course, in order to calculate this explicitly one must express the system in some particular representation. For example, the average value of the x -coordinate of a particle within a state $|\Psi\rangle$ in the $\mathbf{r}$ -representation is given by

$$\langle X \rangle = \int d^3x \Psi^*(\mathbf{x}) \Psi(\mathbf{x})$$

Note that the probability of finding the particle between x and $x+dx$ is given as

$$\langle \Psi(x) | \Psi(x) \rangle dx = \Psi(x)^* \Psi(x) dx$$

so that the expression for $\langle X \rangle$ is the usual definition of the mean value of a random variable with a known probability density in this case given by the scalar product of the associated wavefunction with itself. The wavefunction $|\Psi\rangle$ is also a probability amplitude (not a probability!).

If we now allow the state to evolve in time since in general it is a function of time and since the operator may also be an explicit function of time, we can write a more general expression for the time rate of change of the average value of the observable. This is given as

$$\frac{d}{dt} \langle A \rangle = \frac{1}{i\hbar} \langle [A, H(t)] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle$$

3.4.2. The Root-Mean-Square Deviation.

It can be shown that the rms deviation of a measurement of an observable $\mathbf{A}$ is given by the square root of the average value of the operator $(\Delta\mathbf{A})^2$.

$$\Delta\mathbf{A} = \{ \langle \Psi | (\mathbf{A} - \langle \mathbf{A} \rangle)^2 | \Psi \rangle \}^{1/2}$$

$$\Delta\mathbf{A} = \{ \langle \mathbf{A}^2 \rangle - \langle \mathbf{A} \rangle^2 \}^{1/2}$$

3.4.3. Projection Operators, Projective Measurement, and POVM

Suppose we have a normalized ket $|\Psi\rangle$ and we define an operator (see 2.9.3)

$$\mathbf{P}_\Psi = |\Psi\rangle \langle \Psi|$$

and apply this operator to some arbitrary ket $|\Phi\rangle$ such that

$$\mathbf{P}_\Psi |\Phi\rangle = |\Psi\rangle \langle \Psi | \Phi \rangle$$

This is merely the orthogonal projection of $|\Phi\rangle$ onto the ket $|\Psi\rangle$ since $\langle \Psi | \Phi \rangle$ is merely a scalar product which does not change the direction of $|\Psi\rangle$. $\mathbf{P}_\Psi$ is, therefore, the orthogonal **projection operator** onto the ket $|\Psi\rangle$.

Now if $\mathbf{M}$ is an observable Hermitian operator on a state space with a set of eigenstates $|m\rangle$ and eigenvalues m , then we can write the spectral decomposition of $\mathbf{M}$ as

$$\mathbf{M} = \sum_m m \mathbf{P}_m$$

where the $\mathbf{P}_m$ are projection operators $|m\rangle \langle m|$ onto the eigenspace of $\mathbf{M}$ and the possible outcomes of this **projective measurement** are the eigenvalues of $\mathbf{M}$. The components of this operator are given as an eigenvalue weighted sum of projection operators whose Hilbert Space has a basis that corresponds to the eigenstates of the observable. Also the final state after a projective measurement is an eigenstate of the system. If we make a measurement one of the projection operators.

The above is just a special case of what is known as a **Positive Operator-Valued Measure (POVM)**. In this case we can define an operator

$$\mathbf{E}_m \equiv \mathbf{M}_m^\dagger \mathbf{M}_m \quad \text{such that} \quad \sum_m \mathbf{E}_m = \mathbf{I}$$

where we recall that $\mathbf{M}_m^\dagger$ is the adjoint of $\mathbf{M}_m$. This particular formalism is widely used in QI,

and is useful when one wants to get some insight into the statistics of the measurement. Unlike the projective measurements above, one cannot always infer something about the state being measured.

For example, we may have $\mathbf{M}_1 = a |m\rangle \langle m| + b |m+1\rangle \langle m+1|$ which is essentially a weighted sum of two projective operators/measurements. This is not a projection onto an eigenstate but rather some other state vector in the Hilbert Space. This is a more generalized measurement.

3.4.4. Compatibility of Observables and Commutation Rules.

If we have two observables for the discrete case that are known to commute:

$$[\mathbf{A}, \mathbf{B}] = \mathbf{AB} - \mathbf{BA} = \mathbf{0}$$

Since they commute, they are part of a state space with a common set of eigenkets. This means that for any two eigenvalues of $\mathbf{A}$ and $\mathbf{B}$, a_n and b_m , respectively, there exists at least one state for which a measurement of $\mathbf{A}$ will always give a_n and a measurement of $\mathbf{B}$ will always give b_m . If this is the case, the observables are said to be compatible (i.e. they commute). This is important in quantum information since a measurement of $\mathbf{B}$ following a measurement of $\mathbf{A}$ will not cause any loss of information obtained about $\mathbf{A}$ (and vice versa). If the observables do not commute, then they do not have a common set of eigenkets and simultaneous measurements of $\mathbf{A}$ and $\mathbf{B}$ cannot be made without some uncertainty. According to the Third Postulate, a measurement of $\mathbf{A}$ will place the system in an eigenket of $\mathbf{A}$. An immediately following measurement of $\mathbf{B}$, when the state is an eigenket of $\mathbf{A}$ not common to $\mathbf{B}$, will not give a measure of an eigenvalue of $\mathbf{B}$. This is the main point of the Heisenberg Uncertainty Principle which establishes the commutation relations between non-commuting observables and specifies the error one can expect in this situation.

3.5. Probability Density, and the Probability “Fluid”.

The fourth postulate gave us an expression for finding the probability that a certain measurement will be one of the eigenvalues of the associated observable. If we wish to find the probability that the particle is in a certain state at any point in time we use a different approach.

We will, for purposes of illustration, assume we have a spinless particle with a $\mathbf{r}$ -representation for the state vector which can also be a function of time. The **probability density**, i.e., the probability of finding the particle per unit volume at any time t is given by

$$\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2$$

or the probability of finding the particle at time t in an infinitesimal volume d^3r located at point $\mathbf{r}$ is given as

$$dP(\mathbf{r}, t) = \rho(\mathbf{r}, t) d^3r$$

Now if the particle is subject to some type of scalar potential $V(\mathbf{r}, t)$, the Hamiltonian is given as

$$\mathbf{H} = \mathbf{P}^2/2m + V(\mathbf{R}, t)$$

Upon substituting this into the *Schrödinger* equation with the appropriate substitution of the dynamical variables with their associated operator and applying some mathematical manipulation we can define a probability current as

$$\mathbf{J}(\mathbf{r},t) = \frac{1}{m} \text{Re} \left[\Psi^* \left(\frac{\hbar}{i} \nabla \Psi \right) \right]$$

The local conservation of probability is given by the equation

$$\frac{\partial}{\partial t} \rho(\mathbf{r},t) + \nabla \cdot \mathbf{J}(\mathbf{r},t) = 0$$

This is identical in form to the classical EM theory for the local conservation of electrical charge. If we place the particle in an electromagnetic field, then it is subject to both a scalar and vector potential and the probability current becomes

$$\mathbf{J}(\mathbf{r},t) = \frac{1}{m} \text{Re} \left\{ \Psi^* \left[\frac{\hbar}{i} \nabla - q\mathbf{A}(\mathbf{r},t) \right] \Psi \right\}$$

where $\mathbf{A}(\mathbf{r},t)$ is the vector potential..

It is evident that the above discussion implies, at the quantum level, that there is a sort of **probability “fluid”** that represents the probability of a particle being at a certain point in space at a certain time. We can add to this continuous fluid model a discrete component when we begin to talk about angular momentum and intrinsic spin of a particle at a point in time and space.

3.6 Quantum Interference. Since we define particles as waves, it would seem natural to assume, much like in electromagnetic theory, that there exists interference phenomena between quantum systems which may affect the probability density in the region of interference. One can make an analogy between amplitude of a wave in optics and amplitude of a wave in QM and intensity in optics and probability density in QM. In optics the intensity is given as the modulus squared of the amplitude of the EM field. In QM, the probability density is given as the modulus of the square of the amplitude(state) which is represented by a continuous wave function, i.e., in the $\mathbf{r}$ -representation. To see this more clearly in mathematical terms, let $|u_n\rangle$ be a normalized eigenvector of an observable $\mathbf{A}$ (assume no degeneracy). The probability of finding the eigenvalue a_n when $\mathbf{A}$ is measured when the system is in state $|\Psi_1\rangle$ is given by:

$$P_1(a_n) = \left| \langle u_n | \Psi_1 \rangle \right|^2 \quad \text{and for another orthogonal state } |\Psi_2\rangle \quad \text{we have}$$

$$P_2(a_n) = \left| \langle u_n | \Psi_2 \rangle \right|^2$$

If we now create a normalized state $|\Psi\rangle$ by a superposition of the above two states, then we get

$$|\Psi\rangle = \lambda_1 |\Psi_1\rangle + \lambda_2 |\Psi_2\rangle \quad |\lambda_1|^2 + |\lambda_2|^2 = 1$$

The lambda's are weights (may be complex). To find the probability of measuring the eigenvalue a_n we compute

$$P(a_n) = \left\| \Psi \right\|^2 = \left| \lambda_1 |\Psi_1\rangle + \lambda_2 |\Psi_2\rangle \right|^2$$

which reduces to

$$P(a_n) = |\lambda_1|^2 P_1(a_n) + |\lambda_2|^2 P_2(a_n) + 2 \operatorname{Re} \{ \lambda_1 \lambda_2^* \langle u_n | \Psi_1 \rangle \langle u_n | \Psi_2 \rangle^* \}$$

What this says is that if we have a quantum system whose state is the complex weighted superposition of two orthogonal states, then the probability of measuring a_n is the weighted sum of the probabilities of measuring a_n for each state alone PLUS an added term which is zero only if $\langle u_n | \Psi_1 \rangle$ and/or $\langle u_n | \Psi_2 \rangle$ is zero. Of course, if the λ_i are zero then we have a trivial solution. This interference phenomena for particles plays a central role in the concept of entanglement which is a much researched topic in Quantum Information Technology.

3.7 Quantum Entanglement

In order to simplify the presentation, let us talk only of two quantum systems which are entangled. It is possible, however, that many quantum systems may be mutually entangled. Let us assume that each quantum system is represented in the same basis and that this basis be the binary basis of $|0\rangle$ and $|1\rangle$. Let the two systems be represented by the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$. To represent these as a composite system we merely take the tensor product such that the composite system is now

$$|\Psi\rangle = |\Psi_1\rangle |\Psi_2\rangle \Rightarrow |\Psi_1\rangle \otimes |\Psi_2\rangle$$

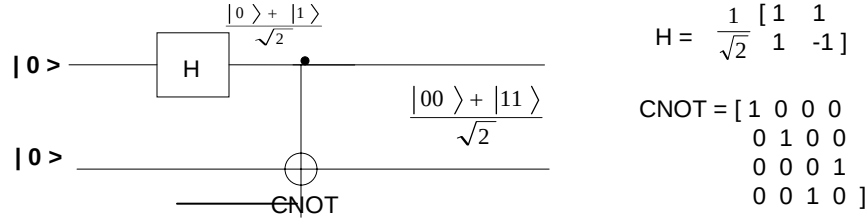
where the adjacent kets $|\Psi_1\rangle$ and $|\Psi_2\rangle$ define the tensor product of the two states without having to use the tensor product symbol $\otimes$. The basis of the composite space is given by the respective tensor products of the basis of the two individual spaces such that

$$|00\rangle = |0\rangle |0\rangle \quad |01\rangle = |0\rangle |1\rangle \quad |10\rangle = |1\rangle |0\rangle \quad |11\rangle = |1\rangle |1\rangle$$

If the composite state cannot be represented by a superposition of the composite basis, we say that $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are entangled. Two areas of QIT research is finding ways to entangle quantum systems and how to measure the degree of entanglement. The physics behind entangling quantum systems is dependent on the type of physical device. Figure 3.1 is a quantum circuit that may be used to establish entanglement regardless of the device.. The resulting state shown in the figure is known as the Bell Basis and is one of the basis kets for the composite system. To create the other 3 basis kets we merely change the inputs of $|0\rangle$ and $|1\rangle$.

Quantum Entanglement and the Bell Basis

Quantum entanglement plays an important role for some quantum applications. As an example start with 2 qubits each in the computational basis $|0\rangle$ and $|1\rangle$ with a composite system computational basis of $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ with each qubit starting out in state $|0\rangle$ (system state $|00\rangle$). Then apply a superposition on the first qubit using a Hadamard operator (matrix) followed by CNOT on the tensor product as follows:



This composite qubit state (also known as an EPR pair after Einstein, Podolski, and Rosen) is said to be entangled.

Figure 3.1. Quantum Circuit for establishing entanglement of two qubits

Of course, Figure 3.1 shows just one possible configuration for an input of $|00\rangle$. The full composite (Bell) basis that may be generated is

<u>Input</u>	<u>Output Bell Basis</u>
$ 00\rangle$	$\frac{ 00\rangle + 11\rangle}{\sqrt{2}}$
$ 01\rangle$	$\frac{ 00\rangle - 11\rangle}{\sqrt{2}}$
$ 10\rangle$	$\frac{ 10\rangle + 01\rangle}{\sqrt{2}}$
$ 11\rangle$	$\frac{ 01\rangle - 10\rangle}{\sqrt{2}}$

3.8 Angular Momentum and Spin

3.8.1 Angular Momentum.³

As we have seen above in section 3.1, the angular momentum of a particle with respect to some origin is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

where $\mathbf{r}$ is the position of a particle with respect to some origin and $\mathbf{p}$ is its linear momentum defined by $m\mathbf{v}$ where m is its mass and $\mathbf{v}$ is its velocity (see figure 3.2a). Notice that a free

particle moving in a straight line can have an angular momentum with respect to some origin but, of course, we are more familiar with the situation where the particle is in some elliptical orbit about some origin which is the source of a central force. Taking the cross product and using the familiar x,y,z coordinates we get

$$L_x = yp_z - zp_y; \quad L_y = zp_x - xp_z; \quad L_z = xp_y - yp_x$$

where the p_x, p_y, p_z are the components of $\mathbf{p}$ on the coordinate axes.

Of course, the corresponding quantum mechanical operator/observable for the angular momentum becomes.

$$\mathbf{L} = \mathbf{R} \times \mathbf{P}$$

and the corresponding components of $\mathbf{L}$ become

$$L_x = YP_z - ZP_y; \quad L_y = ZP_x - XP_z; \quad L_z = XP_y - YP_x$$

or keeping consistent with the symbols used in 3.2.2.

$$L_1 = R_2P_3 - R_3P_2; \quad L_2 = R_3P_1 - R_1P_3; \quad L_3 = R_1P_2 - R_2P_1$$

Using the commutation relations in 3.2.2 between $\mathbf{R}$ and $\mathbf{P}$ we can easily derive commutation relations for the L_i

$$[L_1, L_2] = i\hbar L_3; \quad [L_2, L_3] = i\hbar L_1; \quad [L_3, L_1] = i\hbar L_2$$

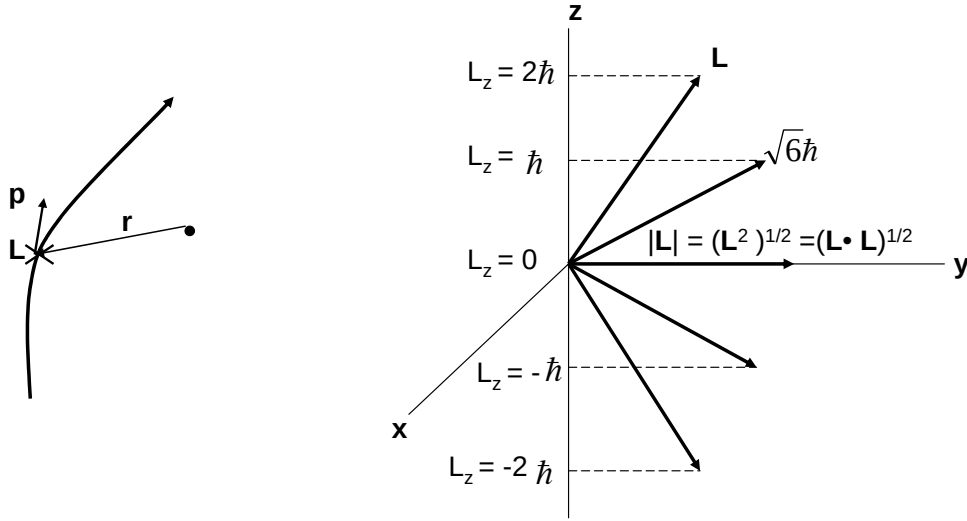
Another angular momentum operator of importance is $\mathbf{L}^2 = L_1^2 + L_2^2 + L_3^2$ which commutes with the angular momentum operator $\mathbf{L}$

$$[\mathbf{L}, \mathbf{L}^2] = 0$$

and as a result commutes with all the components of $\mathbf{L}$. It is also the absolute value squared of the angular momentum. For a free particle ($V(\mathbf{r})=0$), the components of $\mathbf{L}$, $\mathbf{L}^2$, and $\mathbf{H}$ (the Hamiltonian operator) all commute. If the Hamiltonian is a result of a kinetic energy term and a potential $V(\mathbf{r})$, these operators all commute with $\mathbf{H}$ if they commute with $V(\mathbf{R})$ and hence share the same basis.

Since $\mathbf{L}^2$ commutes with the components of $\mathbf{L}$, let us choose L_z . Actually we could have chosen any component or direction but it is “traditional” to use the z-component. It can be shown that

$$\mathbf{L}^2 |l, m_l\rangle = \hbar^2 l(l+1) |l, m_l\rangle \quad l = 0, 1, 2, 3,$$



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Figure 3.2a. Classical particle with linear momentum $\mathbf{p}$ at a distance $\mathbf{r}$ from an origin where the angular momentum vector is into the page

$$L_z |l, m_l\rangle = \hbar m_l |l, m_l\rangle$$

Figure 3.2b. Orientations of the angular momentum vector $\mathbf{L}$ for a quantum particle for $l=2$ and L_z as shown.

$$m_l = -l, -l+1, \dots, l-1, l$$

where $|l, m_l\rangle$ are simultaneous eigenvectors of $\mathbf{L}^2$ and L_z and l and m_l represent quantum numbers which generate the eigenvalues and eigenvectors for $\mathbf{L}^2$ and L_z . Figure 3.2a shows the angular momentum for a classical particle about some reference origin and Figure 3.2b shows the angular momentum for a quantum particle in the states shown. For each discrete value of the magnitude of the angular momentum vector (fixed value of l) there are several discrete projections on the z -axis as shown in figure 3.2b.

We can make a few observations here. First of all, the x and y components of the angular momentum vector are not well defined since the vector can find itself in any cone generated about the z -axis by each vector shown in the figure. There is an uncertainty as to the direction of the vector as a result of the uncertainty in the projections in the x - y plane. This is consistent with the fact that the commutator for L_x and L_y is not equal to zero but is equal to $i\hbar L_z$. Once L_x (or L_y) is measured there will be an uncertainty in the measurement of L_y (or L_x) which increases with increasing values of L_z . This is just one expression of the Heisenberg uncertainty principle. Secondly, we showed that the linear momentum eigenstates of a free particle can be described by plane waves which are not the discrete eigenstates of the angular momentum. However, it can be shown that one can express the eigenstates of linear momentum as superpositions of the eigenstates of angular momentum and vice versa. Hence it doesn't matter which set of

eigenstates we choose to represent a free particle. Therefore both the linear and angular momentum may be expressed using a common basis for the free particle.

3.8.2 Spin

In addition to angular momentum, a particle may have an intrinsic spin. One may ask, “If a particle is a point object, where does spin come into play?”. Particle spin is strictly a quantum mechanical phenomena with no classical analog. When one attempts to measure the angular momentum of a particle, there is a residual amount of angular momentum left over that is not due to the orbital angular momentum about some origin. The spin is considered to be the angular momentum of the particle in its own rest frame. Since there is no classical expression for particle spin, we cannot represent the spin observable with an associated hermitian operator as we did with position and linear and angular momentum but we can postulate that the three components of the spin obey the same commutation relations as the orbital angular momentum and given by³

$$[S_x, S_y] = i\hbar S_z ; \quad [S_y, S_z] = i\hbar S_x ; \quad [S_z, S_x] = i\hbar S_y$$

S^2 and S_z commute and have simultaneous eigenvectors with eigenvalues given by $s(s+1)\hbar^2$ and $m_s\hbar$, respectively, similar to that of the orbital angular momentum and where s and m_s are the quantum numbers as in the orbital angular momentum.

Spin is a very important concept in Quantum Information Technology (QIT). Many of the device technologies being proposed for representing qubits involve the utilization of electron spin and its associated magnetic moment. The complete specification of the state of a particle (i.e. electron) consists of a ket that is a function of position, angular momentum and spin. For the total wavefunction we can denote the following:

$$\begin{aligned} \Psi_+(r) &\text{ represents the wavefunction in } \mathbf{r} \text{ with the electron spin up} \\ \Psi_-(r) &\text{ represents the wavefunction in } \mathbf{r} \text{ with the electron spin down} \end{aligned}$$

and representing the combination of both into a single object written as a column vector

$$\begin{bmatrix} \Psi_+(r) \\ \Psi_-(r) \end{bmatrix}$$

Such a two-component object is referred to as a *spinor* and represents both the spin and the orbital part of the wavefunction for the electron. We can separate these two contributions as follows:

$$\Psi_+(r) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Psi_-(r) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and then define the following spinors as

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We can see how this type of representation can define a set of binary one's and zero's for purposes of computation. In this case χ_+ (spin up) may represent a "1" and χ_- (spin down) may represent a "0". However, in order to be able to compute we need processes to operate on these spins to change their state. It is obvious that these operators may find a representation as 2x2 matrices. Pauli is responsible for a set of 4 matrices called the Pauli Spin matrices given as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

thus defining the vector spin operator (which is Hermitian) as

$$\mathbf{S} = \frac{1}{2} \hbar \boldsymbol{\sigma}$$

with the above three matrices as components of $\boldsymbol{\sigma}$. If we add the 2x2 identity matrix

$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

we get a complete set of 2x2 matrices such that any matrix may be written as superpositions of these matrices. They essentially form a basis for a space of 2x2 matrices. Typical operations are:

$$\sigma_x \chi_+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \quad \sigma_y \chi_{\pm} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \pm i \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \quad \sigma_z \chi_+ = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix};$$

These may be used as single qubit gates in a quantum computer in addition to others. For example, σ_x is a NOT gate changing a "1" to a "0" and vice versa.

In order to physically change the spin state of an electron, it is necessary to interact with it in some way dependent on its physical properties. We know an electron has charge which is how it interacts with electrostatic fields. The electron may have a magnetic moment which interacts with magnetic fields due to its orbital angular momentum but it also has a magnetic moment due to its intrinsic spin. This magnetic moment of the electron may also be represented as an operator (which is Hermitian and also an observable) given by

$$\boldsymbol{\mu} = \frac{e}{m} \mathbf{S}$$

where e is the electronic charge and m is its mass. If the electron is placed in an external magnetic field, the Hamiltonian for this interaction becomes

$$H = -\boldsymbol{\mu} \cdot \mathbf{B}$$

Of course, this leaves out the rest of the Hamiltonian for the electron which depends on its position, velocity (linear momentum) and orbital angular momentum. The orbital angular momentum must also include the effects of the orbiting electron in the magnetic field.

3.9 Quantum Field Theory

Any in depth discussion of this subject would take the scope of this report beyond its original intent. However, since quantum particles and systems change their state as a result of the release or absorption of electromagnetic energy, it is important to have at least a rudimentary knowledge on how this is accomplished.

Quantum field theory was designed to provide a quantum formulation for fields – more specifically the electromagnetic field. The particle which carries the energy of the electromagnetic force is called a photon. At frequencies from zero up to about the Terahertz range it is easier to talk about electromagnetic energy as a wavelike phenomena. However from beyond Terahertz to Infrared, Visible, X-ray, the model for electromagnetic energy is best defined by the photon with energy equal to $h\nu$ where h is Planck's constant and ν is the frequency of the radiation.

The electromagnetic force can be used to control the state of a quantum system that we may want to use in quantum computing. If we wish to make a state transition in a quantum system, we may do so by colliding it with a photon whose energy ($h\nu$) is equal to the difference in energy between the initial state and final state. We shall see in Chapter 5 that the difference between the energy states in the simple one-dimensional harmonic oscillator is $E_0 = \hbar\omega$ ($\hbar = h/2\pi$) so if we wish to increase the state of the oscillator by 1 we need only to supply a photon of energy $h\nu = E_0$. The ω is the angular frequency such that $\omega^2 = k/m$, k is the “spring constant” for the classical harmonic oscillator and m is the mass of the particle. Of course, when the state of the oscillator drops by 1 level then a photon of energy E_0 is emitted. Concepts such as Rayleigh and Raman scattering and Rabi Frequency show how interactions between the EM field and particles (atoms) can take place and the resulting effects of these interactions (See Glossary). These show how photons can be absorbed and then re-emitted at the same or different frequencies depending on the state of the quantum system with which they interact.

See References 32 and 8 (to be looked at first) and 24 for a more in-depth presentation of this topic.

4.0 Information Theory

4.1 Classical Information Theory

4.1.1 Mutual information

Information means many things to many people. However, it is the concept of information as applied to the field of communications and presented by Shannon that we will address here¹. Assume we have a discrete random variable x with an assigned probability distribution $P_X(a_k)$ where the a_k are possible occurrences of the random variable where $k = 1, \dots, K$. The sample space and the probability assignment on the sample space are referred to as an ensemble. We will denote the above ensemble for the sample space as X . In a similar manner we can define an ensemble Y associated with a sample space on the r.v. y with probability assignment $P_Y(b_j)$ for $j = 1, \dots, J$. Let us further assume that both the X and Y ensembles form a joint ensemble denoted by XY with probability assignment $P_{XY}(a_k, b_j)$. With respect to a communication channel, the ensemble X may represent the set of occurrences of an input value $x = a_k$ and the ensemble Y may represent the set of occurrences of an output value $y = b_j$. We can define the information provided about the event $x = a_k$ by the occurrence of the event $y = b_j$ as

$$I_{X;Y}(a_k; b_j) = \log (P_{X|Y}(a_k | b_j) / P_X(a_k))$$

where $P_{X|Y}(a_k | b_j)$ is called the aposteriori probability which defines the probability of an occurrence of $x = a_k$ given an occurrence of $y = b_j$. Therefore, the occurrence of $y = b_j$ changes the probability of $x = a_k$ from the apriori probability $P_X(a_k)$ to the aposteriori probability $P_{X|Y}(a_k, b_j)$. $I_{X;Y}(a_k; b_j)$ is called the **mutual information** between the events $x = a_k$ and $y = b_j$. This definition holds true regardless of what log is used. When a base 2 log is used the units are in bits and when a natural log is used the units are in nats.

The mutual information is also a random variable in the sense that it is a function of the random variables x and y . In that sense we can define a mean, variance, etc. for this random variable. The average or mean of the mutual information is given by

$$I(X;Y) = \sum_{k=1}^K \sum_{j=1}^J P_{XY}(a_k, b_j) \log (P_{X|Y}(a_k | b_j) / P_X(a_k))$$

which is the usual definition of a discrete average being the product of the random variable and its associated probability density function summed over all possible outcomes. In this case we use the joint density function for the two r.v.'s.

4.1.2 Self-Information and Entropy

Another important measure of information is the **self-information**. When the occurrence of a given outcome $y = b_j$ uniquely specifies the outcome of x to be a value a_k , we have the aposteriori probability, $P_{X|Y}(a_k | b_j) = 1$ and

$$I_{X;Y}(a_k; b_j) = \log (1 / P_X(a_k))$$

which is the mutual information required to specify $x = a_k$. We can think of this self-information as the apriori uncertainty of the event $x = a_k$ or the information required to resolve this uncertainty. This self-information can be written as

$$I_X(a_k) = -\log (1/ P_X(a_k)) \quad \text{since it is a function only of the } X \text{ ensemble.}$$

The self-information is also an r.v. and has an average value. This average value is called the **entropy** given by

$$H(X) = - \sum_x P(x) \log P(x)$$

This information entropy is similar to the thermodynamic entropy defined in statistical mechanics and is, in fact, the same under certain conditions which we will not present here.

4.1.3. Distance Measures²

Distance measures in information theory tell us how close two or more ensembles or sample spaces are to each other. How close to the original input ensemble to a system is the output ensemble? A popular distance measure in digital communications is the Hamming distance. However, the Hamming Distance does not lend itself well to Hilbert space representation and so there really is no analog of the classical hamming distance in quantum information.

4.1.3.1. Kolmogorov Distance (L_1 distance)

The Kolmogorov distance is given by the expression

$$D(p_x, q_x) \equiv \frac{1}{2} \sum_x |p_x - q_x|$$

where p_x and q_x represent two separate probability distributions over the same index x .

4.1.3.2. Fidelity

The fidelity is given by the expression

$$F(p_x, q_x) \equiv \sum_x \sqrt{p_x q_x}$$

4.1.3.3. The Relative Entropy

Another measure of closeness between two distributions is the relative entropy. It is defined as relative entropy of $p(x)$ with respect to $q(x)$ and is given by

$$H(p(x) \parallel q(x)) = -H(X) - \sum_x p(x) \log q(x)$$

Its main usefulness lies in the fact that it is a generalization of other entropic quantities and can be used to prove other theorems that concern themselves with entropy.

4.2 Quantum Information Theory²

In quantum information we would like to know how close two quantum systems are to each other in terms of some distance measure. We will look only at the case of discrete systems. As we saw before in Chapter 2, a very useful way to completely specify the state of a quantum system is by using its associated density operator which may be represented as a matrix known as the density matrix. We can define the analog to the classical Kolmogoroff distance as the quantum measure called the Trace distance and a Fidelity criteria for quantum systems.

4.2.1 Trace Distance

The trace distance between two quantum states ρ and σ is defined as

$$D(\rho, \sigma) \equiv \frac{1}{2} \text{tr} |\rho - \sigma|$$

where ρ and σ are the respective density matrices for each state and the trace of the matrix is the sum of the diagonal elements. When $\rho = \sigma$, the trace distance is zero and hence the states are identical. The upper limit being $\frac{1}{2}$ for the case where the diagonal elements of either ρ or σ are zero.

4.2.2. Fidelity

For a quantum state represented by density matrices ρ and σ , the fidelity is given by

$$F(\rho, \sigma) \equiv \text{tr} [\sqrt{\rho^{1/2} \sigma \rho^{1/2}}]$$

When ρ and σ commute, they are diagonal in the same basis and F can be expressed as

$$F(\rho, \sigma) = \sum_i \sqrt{r_i s_i} \quad \text{where } r_i, s_i \text{ are the eigenvalue distributions of}$$

ρ and σ . Recall that in a mixed state, the eigenvalues each have a certain probability of occurrence and hence form a distribution whose values sum to 1.

The density matrix represents a mixed state which is composed of a superposition of pure states. One can show that the fidelity measure of a mixed state with a pure state is given by

$$F(|\Psi\rangle, \rho) = \sqrt{\langle \Psi | \rho | \Psi \rangle}$$

where $|\Psi\rangle$ is a pure state. This is useful in determining the overlap between a pure state and its contribution to a mixed state. Fidelity is also invariant under a unitary transformation.

We can show that there is a relationship between the trace distance and the fidelity. Let $|a\rangle$ and $|b\rangle$ be two pure states. We represent these states in a basis of orthonormal vectors $|0\rangle$ and $|1\rangle$ such that

$$|a\rangle = |0\rangle \quad \text{and} \quad |b\rangle = \cos \theta |0\rangle + \sin \theta |1\rangle$$

We can easily show that $F(|a\rangle, |b\rangle) = |\cos \theta|$ and $D(|a\rangle, |b\rangle) = \sqrt{1 - (F(|a\rangle, |b\rangle))^2}$.

For $\theta = 0$, $F = 1$ and $D = 0$, (the two pure states are identical), and for $\theta = 90^\circ$, $F = 0$, and $D = 1$ (there is a maximum mismatch). The shorter the distance between the states the greater the fidelity and the larger the distance between states the smaller the fidelity.

4.2.3 The Von Neumann Entropy

This is the quantum analog of the Shannon classical entropy. The Von Neumann entropy of a state ρ is given by

$$S(\rho) \equiv -\text{tr}(\rho \log \rho)$$

If λ_x are the eigenvalues of ρ , then we can write

$$S(\rho) = -\sum_x \lambda_x \log \lambda_x$$

Some interesting properties and consequences of the Von Neumann entropy are²

- (1) The entropy is non-negative and is zero if and only if the state is a pure state.
- (2) The maximum value of the entropy in a d-dimensional Hilbert space is $\log d$.
- (3) If the system is in a completely mixed state (i.e. $\mathbf{I}/d$), then the entropy is $\log d$.
- (4) If the system is a composite system AB in a pure state, then $S(A) = S(B)$
- (5) When $|AB\rangle$ is a pure state of a composite system then the $|AB\rangle$ is entangled only if the conditional entropy given by $S(A|B) = S(A,B) - S(B) < 0$
- (6) Projective measurements (see 3.3.3) tend to increase the entropy.
- (7) Generalized measurements (see 3.3.3) can decrease entropy

The entropy of a tensor product $\rho \otimes \sigma$ is $S(\rho \otimes \sigma) = S(\rho) + S(\sigma)$. Note when a state vector in a composite space is not the result of a tensor product of the individual state vectors ρ and σ , we have entanglement and the expression for the entropy is not as given above for the composite state. The two states are not statistically independent so we define a conditional entropy as

$$S(\rho | \sigma) \equiv S(\rho, \sigma) - S(\sigma)$$

and the mutual information as

$$S(\rho : \sigma) \equiv S(\rho) - S(\rho | \sigma)$$

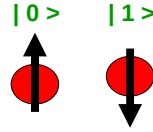
4.3 The Qubit as a Carrier of Information

Most of the work in QIT is presently centered around two state quantum systems. These, in many cases, utilize the two orthogonal spin states of an electron or a photon (see figure 4.1).

Qubits are implemented using Two State Quantum Systems

The focus of some research at this time is the **particle spin states**

Intrinsic Electron Spin (Spintronics)

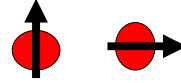


Operations on electron spin states may be accomplished by using the Pauli Spin Matrices for single qubit operations

$$\begin{array}{lll}
 X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} & Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\
 \text{X to Y, Y to X Qubit flip} & \text{Rotation in Hilbert Space} & \text{Reflection}
 \end{array}$$

Where $|0\rangle \rightarrow \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ X-basis $|1\rangle \rightarrow \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ Y-basis

Photon Spin (polarization)



Operations on photon spin states are accomplished using polarizers for single qubit operations

Figure 4.1 Qubits as two state quantum systems

In a classical computer, the lowest level computational basis is “0” or “1”. This is stored as some physical attribute (i.e. magnetic dipole moment, charge, etc) where absence of the attribute may be a “0” and presence would indicate a “1”. We usually refer to these as classical bits. In Quantum Mechanics, however, one can create devices whose physical attributes permit a representation which are a superposition of defined basis states. We refer to these as Quantum Bits or Qubits. Most researched physical attributes today are the spin states of an electron. One can define two basis states of “0” and “1” by setting an electron in its “spin up” state or “spin down” state. But in addition to the classical case, an electron spin state may be in some superposition of both “spin up” (which we will refer to as $|0\rangle$) and “spin down” (which we will refer to as $|1\rangle$). For example we may write a superposition spin state of an electron as

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

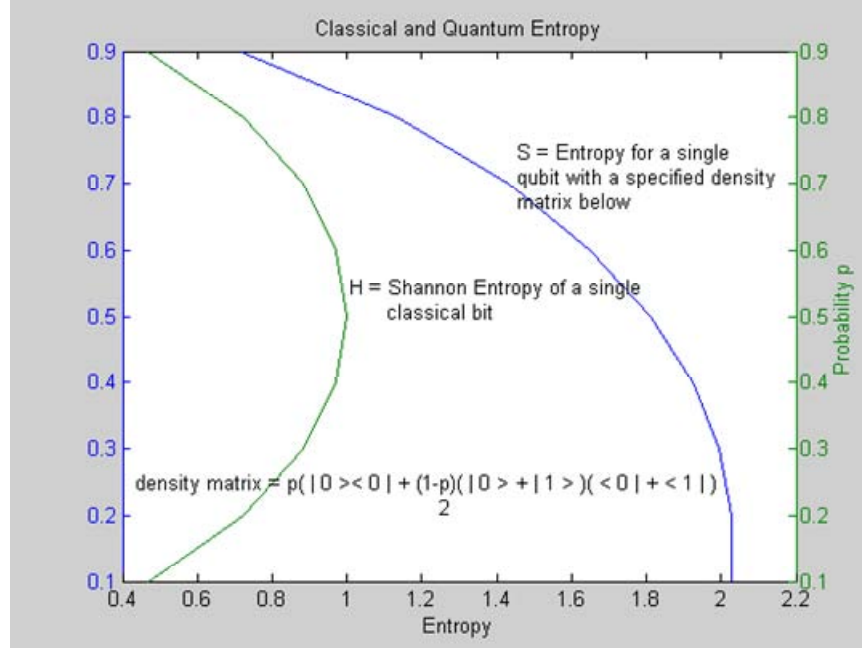


Figure 4.2. Shannon vs. Von Neumann entropy

Finally we can show how superposition can increase the entropy of a single qubit (see Figure 4.2.). As we have stated previously, the state of a qubit represented in a basis of $|0\rangle$ or $|1\rangle$ may also find itself in any superposition of these two basis states. One particular superposition is given as

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

We can specify a system such that the qubit has some probability either being in a state $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$

or a state of $|0\rangle$ and write the density operator/matrix for this as shown in the Figure 4.2. As we have seen in Section 3.3, the density operator contains all the information about the possible states of the system and is used to define Von Neumann (quantum) entropy. This includes the probability of finding the system in these states. Using our definition of the Shannon (classical) entropy and Von Neumann (quantum) entropy given above, we can plot a graph of each of these entropies as a function of the probabilities of occurrence. Here p is the probability of finding the bit or qubit in the state $|0\rangle$ and, of course, $(1-p)$ is the probability of finding the qubit in the state $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$. We note that if the probability of the system being in state $|0\rangle$ is equal to 0.5 then we

have a maximum Shannon entropy of 1 and a Von Neumann entropy of about 1.8. If this were indeed a classical bit ($|0\rangle$ or $|1\rangle$), then the entropy 1 would be maximum. However, if we instead had the possibility for a superposition state given above in the quantum case, we could achieve the value of 1.8. Hence our qubit is capable of storing more information when one of the two possible states is a superposition state. This may not be too surprising since a classical bit is a scalar and is defined only by an amplitude while a quantum bit (qubit) is a vector and may be defined by both an amplitude and a phase.

5.0 Simple Quantum Mechanical Systems³

5.1 The Free Particle

The simplest quantum system is the free particle. DeBroglie defined the frequency and wavelength of a wave that describes a quantum mechanical particle as

$$\nu = E/\hbar \quad \lambda = h/p$$

where ν is the frequency, λ is the wavelength, h is Planck's constant, p is the momentum, E is the particle energy and $\hbar$ is Planck's constant divided by 2π . Of course, the energy is related to the momentum by

$$E = p^2/2m$$

As in classical EM wave theory, we can write an expression for a wave in quantum mechanics as

$$e^{ikx - i\omega t}$$

where the parameters k and ω in QM take on different defining expressions than in classical EM theory. In QM, $k = p/\hbar$ and $\omega = p^2/2m\hbar$.

We can write a wave equation which is the *Schrödinger* Wave Equation for a free particle as

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)$$

Probably the most distinctive difference between a classical wave and a quantum wave is that the speed of a classical EM wave is constant and independent of wavelength whereas the speed of a quantum wave depends on the wavelength and hence is governed by the momentum of the particle. Since one of the basic postulates of QM is that any description of a quantum particle must not be inconsistent with its classical description, and since momentum is mass times velocity, one would expect the speed of a quantum wave packet to be related to the speed of the classical point particle.

Finally, we can write a general solution to the *Schrödinger* Wave Equation as follows:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p,0) e^{i(px/\hbar - p^2 t/2m\hbar)} dp$$

As was shown in section 3.3.1, $\Psi(x,t)$ is a measure of the probability of finding a particle at position x and $x+dx$ at time t or

$$\langle \Psi(x,t) | \Psi(x,t) \rangle dx = \Psi(x,t)^* \Psi(x,t) dx$$

Also the wave function in momentum space, $\Phi(p,0)$, represents the same concept except it is a measure of the probability of finding a particle of momentum p at time $t=0$. Also we can write an expression for $\Phi(p,0)$ as

$$\Phi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ipx/\hbar} dx$$

Since we are assuming a conservative system (constant energy) and no particle interaction, $\Phi(p,0)$ does not change with time. Only $\Psi(x,t)$ changes with time. Not only does $\Psi(x,t)$ represent the wave function of a single free particle but it also is a measure of finding the probability of a particle at any point x at time t of a “wave packet” of many identical particles similar to the concept of a wave packet in EM theory. Likewise, $\Phi(p,0)$ is a measure of finding the probability of a particle with a momentum of p in a wave packet of many identical non-interacting particles.

5.2 Particle in a Potential Well

Above we presented the wave equation for a particle in the absence of a potential. For a particle in a potential, we need to add a term to the Schrodinger Wave Equation to include the possibility of a potential as follows³:

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x) \Psi(x,t) = i\hbar \frac{\partial}{\partial t} \Psi(x,t)$$

where $V(x)$ is the potential at position x .

Whereas, in the case of the free particle, we looked only at the position and momentum of the particle wave, here we look at the possible wavefunctions that are eigenfunctions of the energy operator.

The Hamiltonian for a particle in a potential is given as

$$\mathbf{H} = \mathbf{p}^2/2m + \mathbf{V}(x)$$

where $\mathbf{p}$ and $\mathbf{V}(x)$ are operators as in the $\mathbf{r}$ -representation discussed in 3.2.2. The eigenvalue equation for the energy operator (see 2.10.2) is

$$\mathbf{H} \Psi(x) = E \Psi(x)$$

The time dependence for this can be shown to be of the form $e^{-iEt/\hbar}$. With the proper substitutions for $\mathbf{p}$ we can show that the time independent Schrodinger Wave Equation for the energy is given by

$$-\left[\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi(x) = E \Psi(x)$$

These $\Psi(x)$ are the stationary states of the system. To include the time dependence for the wave function we can show that all we need to do is include the form $e^{-iEt/\hbar}$ as

$$\Psi(x,t) = \Psi(x) e^{-iEt/\hbar}$$

Of course, this additional factor does not change the probabilities since taking the product $\Psi(x,t) * \Psi(x,t)$ is the same as $\Psi(x) * \Psi(x)$ and hence probabilities are time independent.

In the special case where $V(x) = -V_0$ for $|x| < L$ and $V(x) = 0$ for $|x| > L$, we have the problem for what is called a finite square well of constant potential V_0 over a distance of L . The steady state wavefunctions in and around this well are given by

$$\begin{aligned} \Psi(x) &= A \cos\left(\sqrt{2m(V_0 - |E|)} \frac{x}{\hbar}\right) && \text{for } |x| < L \\ &= B e^{-\sqrt{2m|E|} \frac{x}{\hbar}} && \text{for } |x| > L \\ &= B e^{\sqrt{2m|E|} \frac{x}{\hbar}} && \text{for } |x| < -L \end{aligned}$$

It can be shown that the energy eigenvalues are given by the expression

$$\tan \frac{\sqrt{2m(V_0 - |E|)}L}{\hbar} = \frac{-\sqrt{V_0 - |E|}}{\sqrt{|E|}}$$

This needs to be solved either numerically or graphically but it does have discrete solutions for E (see ref 3, pp. 81-82).

As we have seen above, a particle in a finite square well has a finite probability of being outside of the well and the solutions are continuous functions of x , periodic in the well and exponential outside of the well. If we now form a well where $V_0 = \infty$ (see figure 5.1), we can show that the time independent solutions are of the form

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

These represent a set of discrete eigenfunctions (see Figure 5.2) which are eigenfunctions of the energy operator with eigenvalues (see Figure 5.3) and give the discrete energy levels allowed in the well. The energy levels are given by

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2} \quad n = 1, 2, 3, \dots$$

Where m =mass of particle and L is the width of the well.

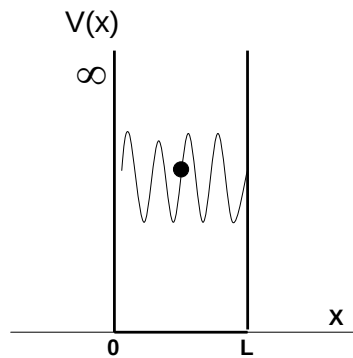


Figure 5.1. Particle in an infinite square well. The particle has no probability of escape no matter how large its Kinetic Energy. Hence the Wavefunction is zero outside the well.

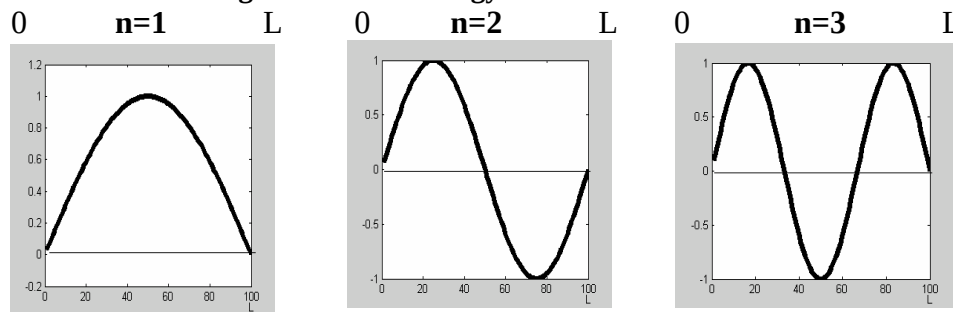


Figure 5.2 First three eigenfunctions for a particle in an infinite square well.

All wavefunctions above $n=1$ have negative values. This is not physically significant since we recall that the probability which is $\Psi\Psi^*$ is what determines the expected position of the particle at any point in space and time.

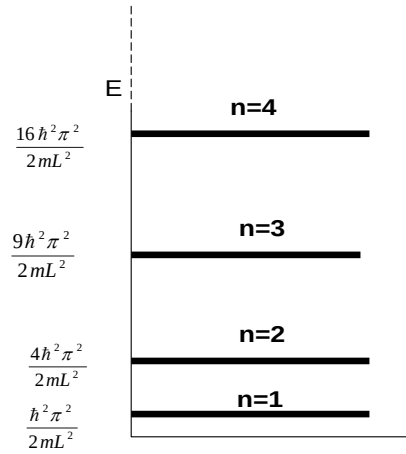


Figure 5.3 Energy-Level diagram for infinite square well for first 4 energy levels

5.3 Particle with a Potential Barrier

A potential barrier is a region where the potential energy is finite inside and zero outside. The Hamiltonian is the same as for the square well but for a constant potential $V(x) = +V_0$ such that

$$V(x) = +V_0 \quad \text{for } |x| < L$$

$$= 0 \quad \text{for } |x| > L$$

The time independent Schrodinger Wave Equation is still

$$-\left[\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi(x) = E \Psi(x)$$

Outside the barrier, where $V(x) = 0$, we have the equation for a free particle whose wavefunction is the sum of the incident and reflected wave for a wave traveling toward the barrier and a transmitted wave after the barrier. Within the barrier, the time-independent Schrodinger Wave Equation becomes

$$-\left[\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_0 \right] \Psi(x) = E \Psi(x)$$

Both the reflectance and transmission of the barrier can be computed in addition to the shape of the wavefunction inside the barrier. Figure 5.4 shows the interaction between a particle of energy $E < V_0$ with the barrier. A potential barrier can be realized by an electron in the

electrostatic field of a central negative charge or in some materials such as GaAs/AlGaAs as we will see when we talk about quantum dots in Chapter 6.

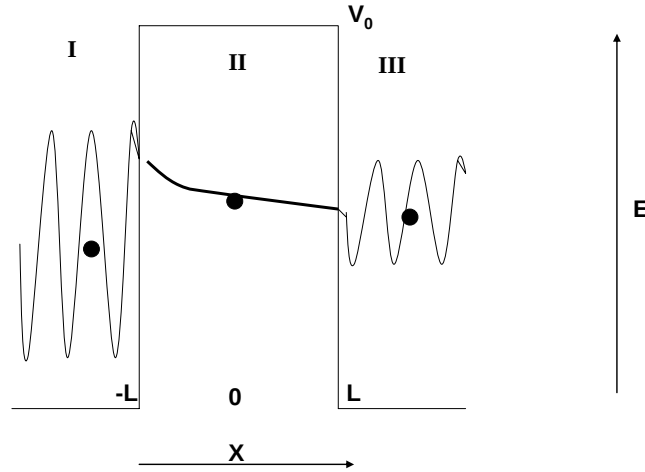


Figure 5.4 Example of the real part of the wavefunction of particle when confronted with a Potential Barrier. The wavefunction is shown in 3 different regions, I , II, and III

5.4 One-Dimensional Quantum Harmonic Oscillator

The theory behind the quantum harmonic oscillator has found applications in developing systems to demonstrate the fabrication of quantum computers and also in the development of the theory of quantum electrodynamics. Quantum Electrodynamics (QED) is used to define quantum states of electromagnetic waves and the quantum harmonic oscillator is just one method by which states are defined. QED also permits the modeling of particle/EM wave interactions using a single unified quantum approach. Lasers (photons) are one method used to control the states of quantum systems of matter particles such as electrons in QI devices. We will present just the 1-D case. As might be presumed, when we get into higher dimensions things get more complex and we also create degenerate states due to the symmetries of the geometry.

The classical 1D harmonic oscillator Hamiltonian is given as³

$$H = p^2/2m + \frac{1}{2} m\omega^2 x^2$$

where ω is the angular frequency such that $\omega^2 = k/m$ and the second term is the potential. The constant k is the “spring constant”.

As an operator in quantum mechanics it is

$$\mathbf{H} = \mathbf{p}^2/2m + \frac{1}{2} m\omega^2 \mathbf{x}^2$$

Where, as above, both $\mathbf{p}$ and $\mathbf{x}$ may be operators in the $\mathbf{r}$ -representation. The time independent eigenvalue equation again is

$$\mathbf{H} \Psi(x) = E \Psi(x)$$

and with proper operator substitution results in the differential equation

$$-\left[\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \Psi(x) = E \Psi(x)$$

Unlike the potential well and barrier problems above, this system has a bit more complex potential $V(x)$ and the solutions will also be more complex. In fact, the wavefunctions of the energy eigenstates are

$$\Psi_{En}(x) = \frac{1}{2^{n/2}} \frac{1}{\sqrt{n!}} \frac{1}{\sqrt{x_0} \sqrt[4]{2\pi}} e^{-\frac{1}{2}\zeta^2} H_n(\zeta)$$

where $H_n(\zeta) = n^{\text{th}}$ order Hermite Polynomial

$$\zeta = x/x_0$$

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

The energy eigenvalues associated with these eigenstates are given by

$$E_n = \hbar \omega (n + \frac{1}{2})$$

See Figure 5.5.

We can also represent the Hamiltonian operator of the 1-D harmonic oscillator in terms of two operators $\mathbf{a}$ and $\mathbf{a}^\dagger$ where $\mathbf{a}^\dagger$ is the adjoint of $\mathbf{a}$ (see 2.9.4) and are defined as follows:

$$\mathbf{a} = \frac{1}{\sqrt{2}} (\mathbf{x} + i\mathbf{p}) \quad \mathbf{a}^\dagger = \frac{1}{\sqrt{2}} (\mathbf{x} - i\mathbf{p})$$

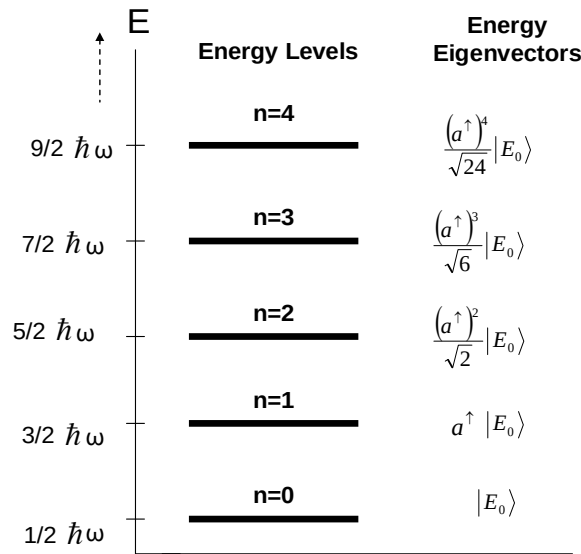
where again $\mathbf{x}$ and $\mathbf{p}$ are the position and momentum operators in the $\mathbf{r}$ -representation. The Hamiltonian operator is then given by

$$\mathbf{H} = \hbar \omega (\mathbf{a}^\dagger \mathbf{a} + \frac{1}{2})$$

The operators $\mathbf{a}$ and $\mathbf{a}^\dagger$ are referred to as the lowering and raising operators, respectively. When they operate on an eigenstate, they lower or raise the state by one level. For example

$$\mathbf{a}^\dagger \Psi_{E_0}(x) = \Psi_{E_1}(x) \quad \text{and} \quad \mathbf{a} \Psi_{E_1}(x) = \Psi_{E_0}(x)$$

These operators play an important role in defining electromagnetic quantum states in Quantum Field Theory⁸. For example, if you wish to raise the state of the system from the ground state to the first excited state, you just apply a raising operator, $\mathbf{a}^\dagger$. Figure 5.5 shows the first five energy eigenvalues of the harmonic oscillator starting with the ground state $|E_0\rangle$. The effect of the raising operator on the previous state is shown.



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Figure 5.5 Energy Levels and Eigenvectors for the first five energy eigenstates (with normalizing constants) of a harmonic oscillator.

The corresponding eigenfunctions for the first four states ($n=0, 1, 2, 3$) are shown in figure 5.6. In this figure the variable

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}$$

All wavefunctions above $n=0$ have negative values. This is not physically significant since we recall that the probability which is $\Psi\Psi^*$ is what determines the position of the particle.

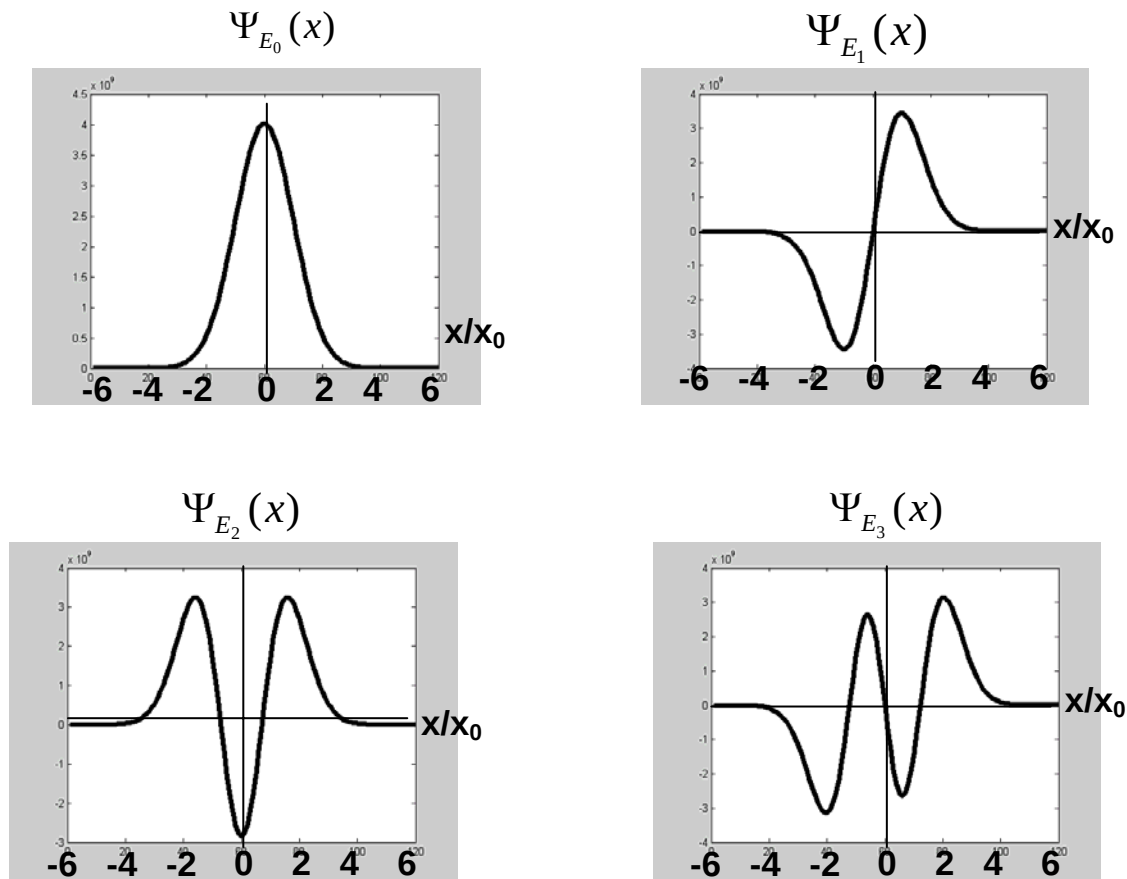


Figure 5.6 Eigenfunctions for the first 4 eigenstates of a 1-D Quantum Harmonic Oscillator

6.0 Physical Implementations

6.1 The Penning Trap (geonium atom)⁷

The Penning trap is a device which permits the trapping of an electron or swarms of electrons in a confined space for which may be used as quantum states for quantum information processing. In nature, the nuclei of atoms perform this function from Hydrogen (with one electron) and up the periodic table for many nuclei/electron atomic systems. The type of quantum system implemented by the Penning trap is referred to as a “geonium atom” since the electrons are controlled by a physical device bound to the Earth rather than a negative electrostatic potential provided by the nucleus in natural atoms.

Unlike a natural atom, the potential fields in the Penning trap are a homogeneous magnetic field (vector potential) and a quadrupole electrostatic potential. A diagram of the fields within the trap is shown in figure 6.1. The homogeneous magnetic field $\mathbf{B}$ is shown pointing in the z direction for both Figs 6.1 and 6.2. There are three types of motion defined in this situation: the magnetron motion which is a large circle in the xy plane; the axial oscillation

which is sinusoidal in the z direction; the cyclotron motion which is a circular motion about the path of the axial oscillation (see figure 6.2).

The electrostatic quadrapole potential is given by ⁹

$$V = V_0 \frac{x^2 + y^2 - 2z^2}{4d^2}$$

where d characterizes the dimension of the trap and V_0 is the potential applied to the trap electrodes shown in Figure 6.1. Along with the applied magnetic field one can write the Hamiltonian for an electron trapped in these fields as

$$H = \frac{1}{2m} [\mathbf{p} - e \mathbf{A}]^2 + eV - \frac{g}{2} \frac{e\hbar}{2m} \boldsymbol{\sigma} \cdot \mathbf{B}$$

where g is the electron's g factor and

$$\mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r} + \mathbf{A}_{\text{ext}}$$

The g factor is a constant which expresses the electron's magnetic dipole moment in terms of its spin angular momentum¹⁰. The position and conjugate angular momentum operators are given by $\mathbf{r}$ and $\mathbf{p}$, respectively, and $\boldsymbol{\sigma}$ are the Pauli spin matrices σ_x , σ_y , σ_z . If we eliminate any external vector potentials, $\mathbf{A}_{\text{ext}}$, then the motion of the electron is determined by the motion of three harmonic oscillators, the cyclotron, the axial and the magnetron in addition to a electron spin precession about the z axis. As we did with the harmonic oscillator in Chapter 5, we can introduce the raising and lowering operators (sometimes referred to as ladder operators) in this case being $\mathbf{a}_z$, $\mathbf{a}_c$, and $\mathbf{a}_m$, one for each of the three motions, axial, cyclotron, and magnetron. As in the simple 1-D harmonic oscillator these operators are expressed in terms of the $\mathbf{r}$ and $\mathbf{p}$ ($\mathbf{r}$ -representation) operators and with some effort the Hamiltonian may be expressed as

$$\mathbf{H} = \hbar \omega_z \mathbf{a}_z^\dagger \mathbf{a}_z + \hbar \omega_c \mathbf{a}_c^\dagger \mathbf{a}_c - \hbar \omega_m \mathbf{a}_m^\dagger \mathbf{a}_m + \frac{\hbar}{2} \omega_s \sigma_z$$

where the angular frequencies are given as

$$\omega_z = \sqrt{\frac{|e| V_0}{m d^2}}, \quad \omega_c = \frac{|e| B}{m}, \quad \omega_m \approx \frac{\omega_z^2}{2\omega_c}, \quad \omega_s = g |e| B / 2m \text{ (spin precession freq.)}$$

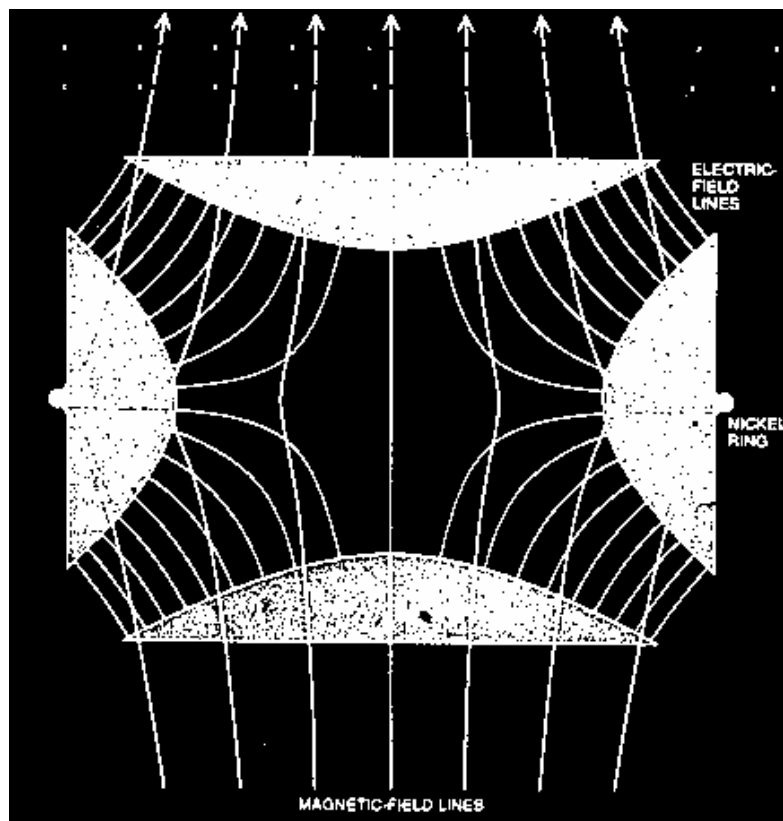


Figure 6.1 Penning Trap (From Ekstrom and Wineland¹¹)

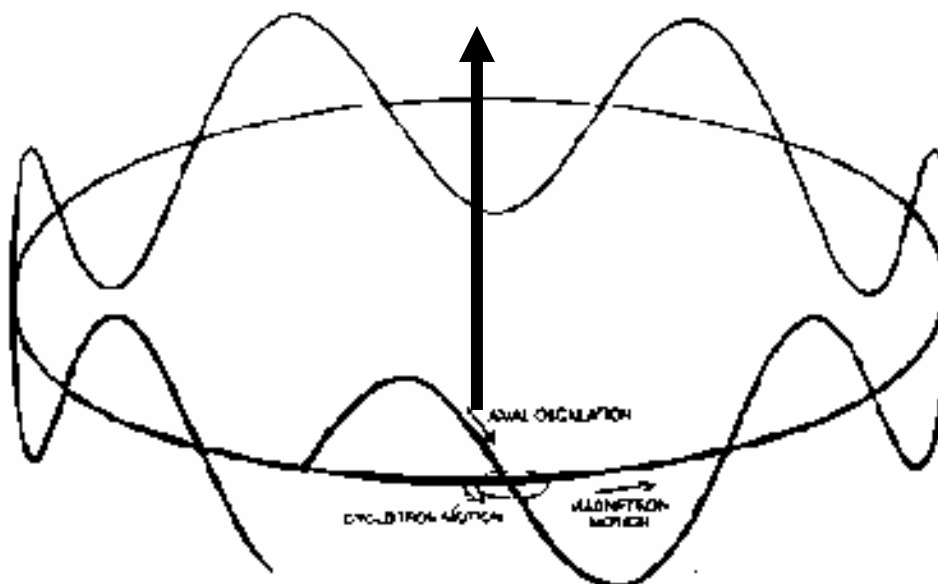


Figure 6.2 Motion of electron in Penning trap (From Ekstrom and Wineland¹¹)

Typically, $\omega_z/2\pi$ is in the MHz range, $\omega_c/2\pi$ is in the GHz range, and $\omega_m/2\pi$ is in the kHz range.

The above development addresses four possible degrees of freedom of an electron in the Penning trap. Each degree of freedom, cyclotron, axial, magnetron, and spin has associated with it a set of discrete energy levels resulting from the discrete angular frequencies in each case. The first three terms in the above Hamiltonian have solutions of their respective eigenvalue equations which are 1-D harmonic oscillators in each of the three degrees of freedom.

Let us now apply an external vector potential field $\mathbf{A}_{\text{ext}}$ which is a standing wave along the z direction and circularly polarized in the x-y plane with a frequency Ω . It has a sinusoidal nature in the x and y directions and no component in the z direction. A phase factor in the expression for this field defines the position of the center of the axial motion with respect to the standing wave and its value can be used to position the electron anywhere between a node and an antinode. It can be shown that for frequencies Ω close to ω_c and ω_s , the slow magnetron motion can be ignored and the approximated Hamiltonian is no longer a function of the magnetron motion.

To represent two qubits, we consider only the spin and axial degrees of freedom, respectively. It can be shown that this particular Penning trap based on the “geonium atom” concept may be used to implement a control-not gate. In this case the spin is the “target” qubit and the axial degree of freedom is used as the “control” qubit. The system is prepared in such a way that it is deep cooled to the ground states of the axial and cyclotron oscillations and the two states, axial and spin, are entangled resulting in a truth table for the C-Not gate as follows:

$$\begin{aligned} |0\rangle_z |\downarrow\rangle &\rightarrow |0\rangle_z |\downarrow\rangle \\ |0\rangle_z |\uparrow\rangle &\rightarrow |0\rangle_z |\uparrow\rangle \\ |1\rangle_z |\downarrow\rangle &\rightarrow |1\rangle_z |\uparrow\rangle \\ |1\rangle_z |\uparrow\rangle &\rightarrow |1\rangle_z |\downarrow\rangle \end{aligned}$$

Due to this entanglement, the electron spin state or “target” qubit is not affected by a change in the axial ground state. However, whenever the axial state is elevated by one level to a $|1\rangle_z$, then it flips the state of its entangled spin state.

6.2 Quantum Dots, Quantum Wells, and Quantum Wires

Quantum dots are small regions that are capable of confining quantum systems. Using quantum dots, one can create “artificial atoms”. In a natural atom, the electrons are bound by a spherically symmetric central potential which is supplied by the electrostatic charge of the nucleus. Since natural atoms are 3-dimensional, 3-D degeneracies arise which yield the many electron shells which the beginning physics/chemistry student is familiar with. Each cell represents a fixed energy with each electron in the shell in a unique state but all with the same energy (hence the degeneracy). Each filled shell may contain only a maximum number of electrons starting with 2 electrons in the first shell and 10, 18, 36, etc. for each succeeding outer shell. For example, Quantum dots as artificial atoms, having a disc shape with only 2-D symmetries, have an electron shell structure with 2, 6, 12, 20, electrons in respective shells.

A good example on how one might fabricate a quantum well, quantum wire, or quantum dot can be shown using a heterostructure consisting of GaAs and AlGaAs¹². Figure 6.3 is an

approximate representation of the respective energy bands. Figure 6.4 shows a slab of GaAs sandwiched between two slabs of AlGaAs. The AlGaAs on either side of the GaAs forms a high potential barrier trapping the GaAs conduction band electrons in a square well in the y-direction. In the x-z direction the electron's wave function may be approximated by that for free electrons with an effective mass given by that of an electron in a GaAs lattice (see section 5.1).

As we noted in section 5.2 which discusses the square well, the energy levels of an electron trapped in a square well are discrete but do not have an analytical solution. To find them we need to use either numerical or graphical methods. Let us assume for this discussion that the square well is not finite but rather is infinite. In this case, we showed at the end of section 5.2 that we can obtain an analytical expression for the energy levels of the electron in an infinite square well given by¹²

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

Figs. 5.2 and 5.3 in Section 5.2 shows diagrams of the respective eigenfunctions and eigenvalues.

For a quantum well as shown in Fig. 6.4, the thin layer in the y-direction gives rise to a square potential well for the conduction band electrons. The width of the well should be smaller than the deBroglie wavelength of the electron or

$$\lambda = \frac{h}{p}$$

where $p = m_n v$ and m_n is the effective mass of the electron and v is its velocity. Since we wish the quantization levels to be effective, the electron should have an energy which is much less than $k_B T$ where k_B is the Boltzman constant and T is the temperature in degrees Kelvin. This is essentially the thermal energy of the electron. Using the results for an infinite square well as an approximation, the lowest energy levels for a square well in such a structure is approximately

$$E_j - E_c = \frac{\pi^2 \hbar^2}{2m_n L^2} j^2$$

Where L is the width of the square well and j is the quantum number labeling the energy levels. In the y-direction (inside the 1-dimensional well), the electron is confined to only certain discrete states and forms a 2 dimensional electron gas. In the x-direction, however, the electron is allowed to move freely and its wave function is approximated as a free particle (see Section 5.1). In fig. 6.5 we have a “quantum wire” which, supports the free particle wave function in x and in the y-and z-direction the discrete states may be used to hold information. The particle wave is broad in the x-direction but is confined in the y-z direction.

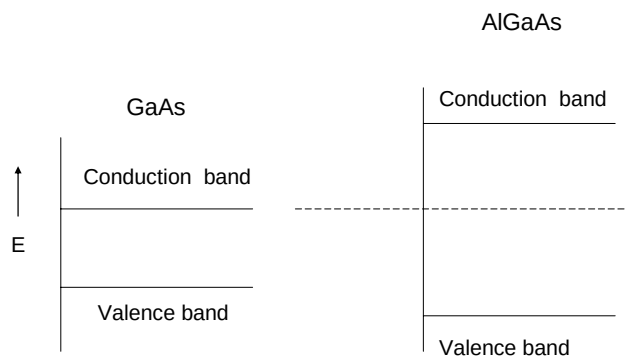


Figure 6.3 Energy band diagrams for GaAs and AlGaAs

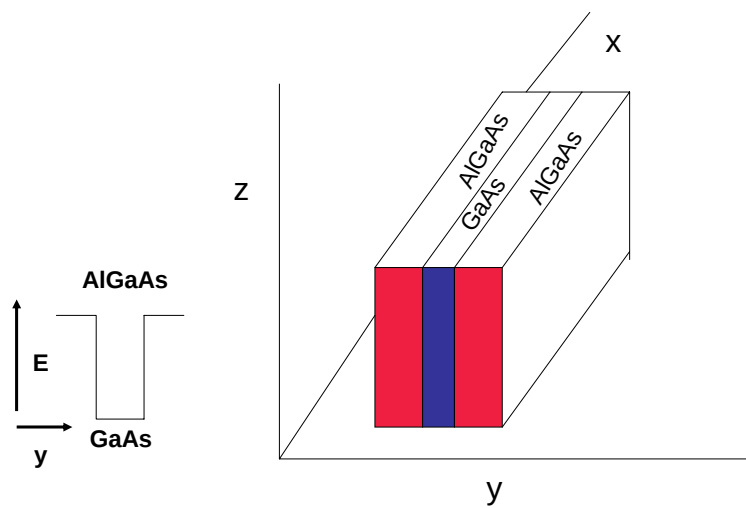


Figure 6.4 One Dimensional Quantum Well

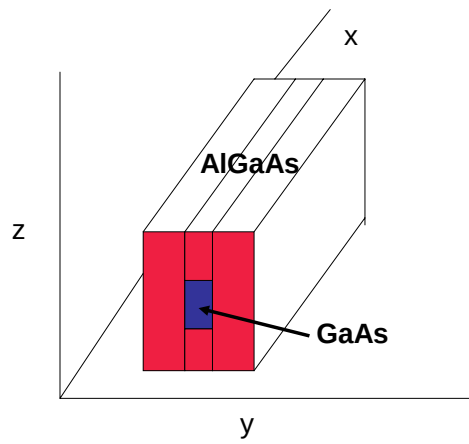


Figure 6.5 Quantum Wire

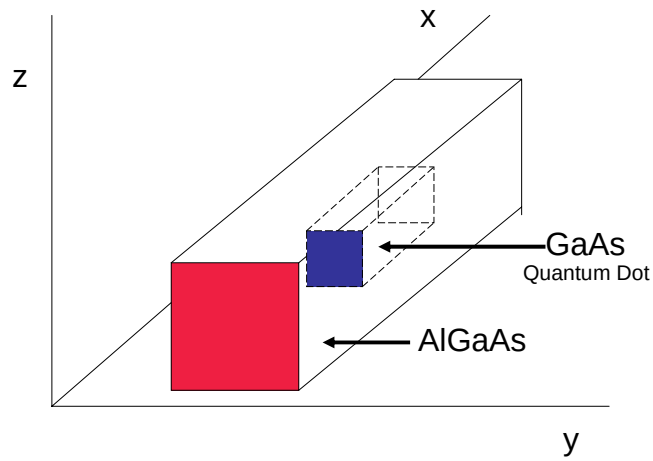


Figure 6.6. Quantum Dot

If we now surround the GaAs completely with AlGaAs (see Fig. 6.6), we form a box which we call a quantum dot. An electron trapped in this quantum dot now can only assume certain energy levels which are given by

$$E_n = \frac{\pi^2 \hbar^2}{2m} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right) \quad n_1, n_2, n_3 = 1, 2, 3$$

and a, b, c are the dimensions of the rectangular box in x, y , and z . Also here we assume that the periodic potential of the crystal lattice does not affect the energy of the electron and we use the value for the rest mass m rather than the effective mass m_n . We can see that the quantum dot may be used for storage of information while the quantum wire may be used to transport information.

This has been a very simplistic example since actual devices for information storage and transport being developed today tend to be more complicated. However, this example does illustrate how solid state materials and quantum systems of particles such as electrons can be used for storage and retrieval of information. Other interesting and related quantum dot approaches can be found in references [13-19].

7.0 Quantum Algorithms

7.1 Grover's Search Algorithm^{20,25}

This algorithm is useful for performing database search for unsorted databases. Let assume we have a database of N items. The database is represented by a set of numbers in a table such that $x \in \{0, 1, 2, \dots, N-1\}$. We can define an "oracle" such that

$$|x\rangle \xrightarrow{O} (-1)^{f(x)} |x\rangle$$

Where O is the operation of the Oracle on the vector $|x\rangle$ and $f(x)=1$ if $|x\rangle$ is a solution and $f(x)=0$ if $|x\rangle$ is not a solution. Therefore the Oracle will reflect all vectors that are solutions.

The algorithm can be seen more clearly using a geometric visualization². Assume we have an n qubit register. We can define an Oracle (a unitary operator) as

$$O = 2|0\rangle\langle 0| - I$$

where $|0\rangle$ is the zero state of the n qubit register which can be represented by an $n \times 1$ matrix =

$$\begin{bmatrix} 0 \\ 0 \\ | \\ | \\ 0 \end{bmatrix} \quad \text{and} \quad O(n \times n) = \begin{bmatrix} -1 & 0 & \dots & 0 \\ 0 & -1 & \dots & 0 \\ \dots & 0 & \dots & \dots \\ \dots & \dots & 0 & -1 \end{bmatrix}$$

I is the $n \times n$ identity matrix

Let us define two normalized states

$$|\alpha\rangle = \frac{1}{\sqrt{N-M}} \sum_x^{nsol} |x\rangle \quad \text{the sum over all } |x\rangle \text{ which are not solutions}$$

$$|\beta\rangle = \frac{1}{\sqrt{M}} \sum_x^{sol} |x\rangle \quad \text{the sum over all } |x\rangle \text{ which are solutions}$$

$N = 2^n$ = total number of possible register states

M = total number of states that are solutions

$|x\rangle$ = any one of 2^n possible states for the register

It can be shown that the initial state of the quantum computer is in the space spanned by

$|\alpha\rangle$ and $|\beta\rangle$ (see figure 7.1). The initial state can now be expressed as

$$|\Psi\rangle = \sqrt{\frac{N-M}{M}}|\alpha\rangle + \sqrt{\frac{M}{N}}|\beta\rangle$$

One can define an operator G known as the Grover iteration operator as

$$G = 2|\Psi\rangle\langle\Psi| - I$$

Applying the Oracle to an input vector reflects the vector about $|\alpha\rangle$. Following this by applying the operator G rotates $O|\alpha\rangle$ about $|\Psi\rangle$ by an amount θ .

The angle θ in figure 7.1 is computed using $\theta = 2 \times \arccos\left(\sqrt{\frac{N-M}{N}}\right)$

Successive iterations by G continue to rotate the resultant vector by G. This iteration must occur R times before the input vector is rotate to coincide with $|\beta\rangle$ or close to $|\beta\rangle$.

$$R = \text{CI}\left(\frac{\arccos\sqrt{M/N}}{\theta}\right) \text{ where CI is a halves down round off.}$$

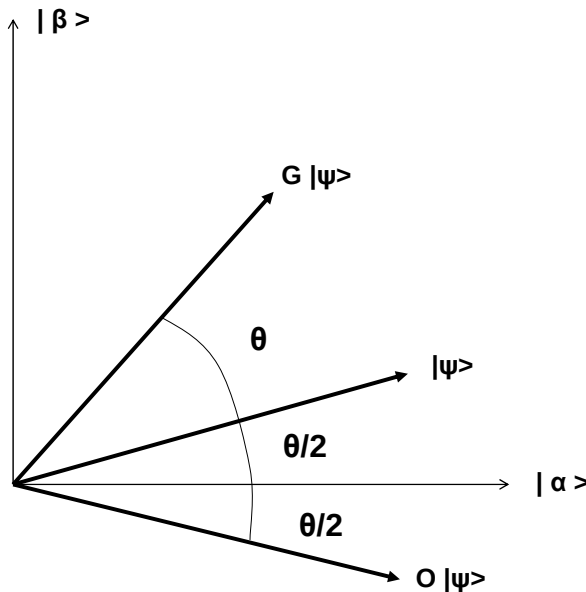


Figure 7.1 Geometric representation of Grover iteration2

As an example, let us apply this algorithm to finding a specific pixel value in an image. For simplicity we can use the simple 4-bit linear image array shown in figure

7.2. Let us perform the following:

1. We construct our G operator for the case where we are searching for a pixel value of 4. We therefore have only one solution vector $x = 4$ and use this to fix $|\beta\rangle$
2. We compute the value of R and we find that it is 3.
3. We perform 3 iterations using G.
4. One way to measure the closeness of $G^3|4\rangle$ and $|\beta\rangle$ is take their scalar product. The value of the scalar product will be close to 1 if there is a match and will be much less than 1 if there is not a match. This also can be considered a measure of the probability. Below is a table of the probability measures for the first 4 pixels in the image shown in the figure

<u>Pixel value</u>	<u>Probability Measure</u>
10	0.3638 (miss)
1	0.2143 (miss)
4	0.8998 (hit)
2	0.2143 (miss)

If we perform these searches on a classical computer we have to perform on the average $N/2$ or 8 search operations per pixel. On the quantum computer it takes only about 3 iterations of the Grover operator plus one for the Oracle or a total of $4(\sqrt{N})$.

The probabilities appear to never be 1 or 0 but the hit versus miss probabilities are so far apart that one could easily establish an upper and lower threshold to detect a hit or a miss.

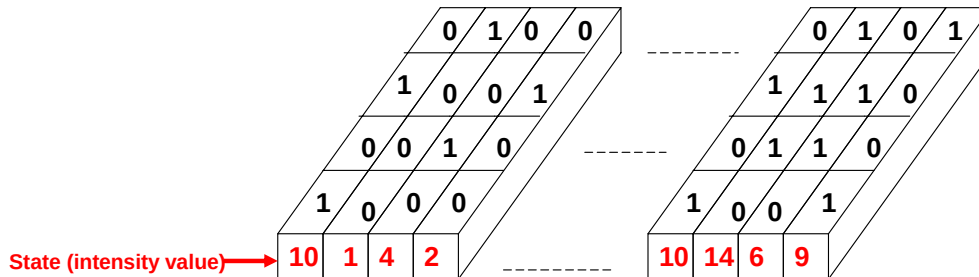


Figure 7.2 Simple linear 4-bit image array showing pixel values in red

7.2 Superdense Coding

A good example of information processing tasks that may be accomplished using quantum mechanics is superdense coding². We have seen in section 4.3 how a single qubit may carry more information than a classical bit if we use the concept of superposition in establishing one state of the qubit or what is referred to as the Bell Basis. In section 3.6 we showed how we could create the Bell Basis using the process shown in the circuit diagram of Figure 7.3. Figure 7.4. gives a possible implementation using quantum dots to confine and operate on the two state electron spin.

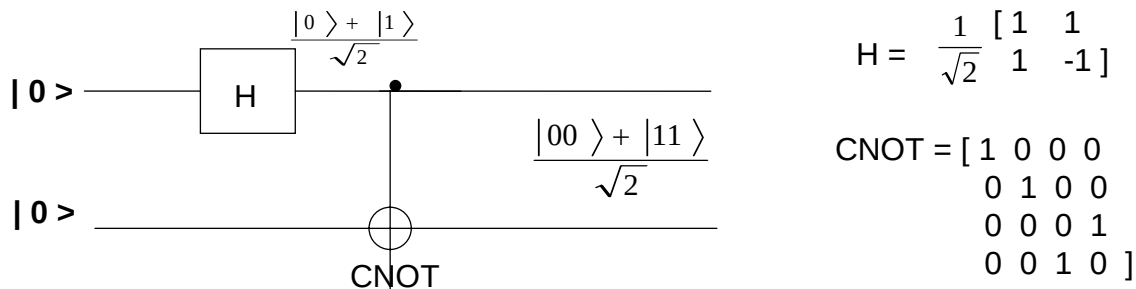


Figure 7.3 Circuit for creating Bell Basis

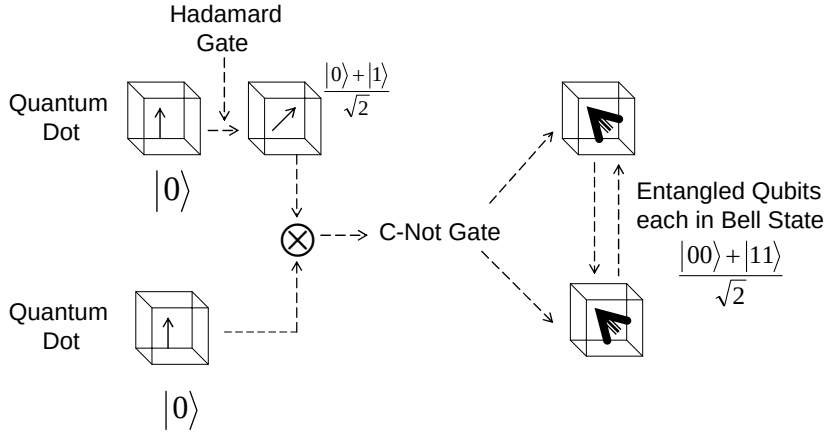


Figure 7.4 Entangling two electron spin qubits each confined by a quantum dot

In the above figure, we start with a system of two electrons each confined by a quantum dot and each initially in the spin-up state. Of course, any two-state system or any two states of a multiple state system would be appropriate for this application assuming one can fabricate the devices necessary to perform the functions required. The system starts out in the composite $|00\rangle$ state.

The upper qubit is multiplied by the Hadamard Gate/Matrix. Physically, this may be some process that changes the potential within the quantum dot and hence changes the spin state of the electron. One may also apply a magnetic field that interacts with the magnetic moment of the electron. In any case, this physical operator that is applied must be represented by a matrix that looks like the Hadamard matrix shown in figure 7.3. The composite state is now given as

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle = \frac{|00\rangle + |10\rangle}{\sqrt{2}}$$

This is not the desired entangled Bell State so we follow this by a CNOT operation whose matrix is shown in figure 7.3. In matrix representation we have

$$\text{Bell}(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right] = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \Rightarrow \text{"00"}$$

Likewise we can show

$$\text{Bell}(1) = \frac{|00\rangle - |11\rangle}{\sqrt{2}} \Rightarrow \text{"01"}; \quad \text{Bell}(2) = \frac{|10\rangle + |01\rangle}{\sqrt{2}} \Rightarrow \text{"10"};$$

$$\text{Bell}(3) = \frac{|01\rangle - |10\rangle}{\sqrt{2}} \Rightarrow \text{"11"}$$

The above is a complete set of basis functions for the composite space and is referred to as the Bell Basis.

We have now laid the groundwork for showing superdense coding. Let us give one qubit to Alice and the other one to Bob. Alice wishes to communicate one of the four Bell states representing the digits 0,1,2,3. She could send 2 bits over a classical channel and be done with it but she has available to her some information that Bob also has, i.e., a qubit representing Bell State (0). Rather than using 2 bits over a classical channel, she chooses to send just one qubit over a quantum channel. To do this she needs the following gates (see section 3.7.2 for the Pauli Spin matrices):

$$\text{Identity gate} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\text{Pauli Z gate} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\text{Quantum NOT gate} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$i * \text{Pauli Y gate} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

where “i” is the imaginary $\sqrt{-1}$

Since her qubit resides in the composite space resulting from the tensor product of the individual basis for each of the original unentangled qubits, she needs to represent these matrices in this composite space using the extension procedure given in section 2.10.5

$$\text{Extended Identity gate} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\text{Extended Pauli Z gate} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\text{Extended Quantum NOT gate} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\text{Extended } i * \text{Pauli Y gate} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

If she wishes to send a “00” then she applies the Extended Identity matrix to her qubit and sends the result. In other words, she does nothing to her shared qubit with Bob. If she wishes to send a “01” she applies the Extended Pauli Z gate to her qubit such that

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] = \text{Bell}(1) \rightarrow \text{“01”}$$

If she wishes to send a “10” she applies the Extended Quantum NOT gate to her qubit such that

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] = \text{Bell}(2) \rightarrow \text{“10”}$$

If she wishes to send a “11” she applies the Extended $i * \text{Pauli Y}$ gate to her qubit such that

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right] = \text{Bell}(3) \rightarrow \text{“11”}$$

So Alice can communicate two classical bits of information using just one qubit of quantum information. Physically, this communication can be accomplished using quantum wires as was presented in Chapter 6 from one storage location to another (i.e., one quantum dot to another).

The above process is mathematically straightforward but actual physical implementation of the gates and storage of data is not so easy. Much of the research in experimental quantum

mechanics/information focuses on how one physically fabricates the necessary quantum gates, how to interface them with storage devices, and building storage devices such as quantum dots that may support a quantum state long enough to effect an operation and read out the results. The read out process is also a challenge due to phenomena such as “decoherence” (quantum equivalent of classical noise) which destroys the desired state of a quantum system and “wave function collapse”, which collapses the quantum system into one of its several eigenstates upon making a measurement on the system. The Bell Bases are not eigenstates of the electron spin in the above case but rather derived from a superposition of these eigenstates and once a state is established it must persist long enough for a calculation to be made. One of the causes of decoherence comes from the fact that the system is not completely isolated and is subject to external stochastic potentials such as the quantum EM field background (photons). Also, after the measurement is made, the state of the spin drops into one of its eigenstates and the information is lost. These are just some of the many issues confronting the Quantum Mechanics/Information research community.

8.0 Summary and Conclusions

8.1 Summary

Figure 8.1 gives a summary comparison of a classical and quantum system. One of the major differences is the fact that the state of a quantum particle may have both an amplitude and phase whereas the state of a classical particle has only one scalar value to represent its state.

<u>Classical System</u>	<u>Quantum System</u>
Smallest indivisible unit of matter is a point particle	Classical particle represented by a wavefunction
Dynamics expressed by Newtons classical mechanical laws governing systems of point particles	Schrodinger Wave Equation completely defines the dynamics of a system of particles.
Measureable system variables such as energy, momentum, position of particles are deterministic, continuous, with scalar components.	Measureable system variables such as energy, momentum, position of particles are indeterministic , may be continuous or discrete, and have both amplitude and phase due to their wavelike nature.
The position of a classical particle is exactly determined as occupying an exact position in space.	The position of a quantum particle is spread out in space as determined by the extent of its wavefunction

Figure 8.1 Classical versus Quantum Systems

Figure 8.2 outlines how we can use a classical formulation of the dynamics of a particle to write a differential equation (Schrodinger Wave Equation) whose steady state solutions represent the various states of a quantum particle/system.

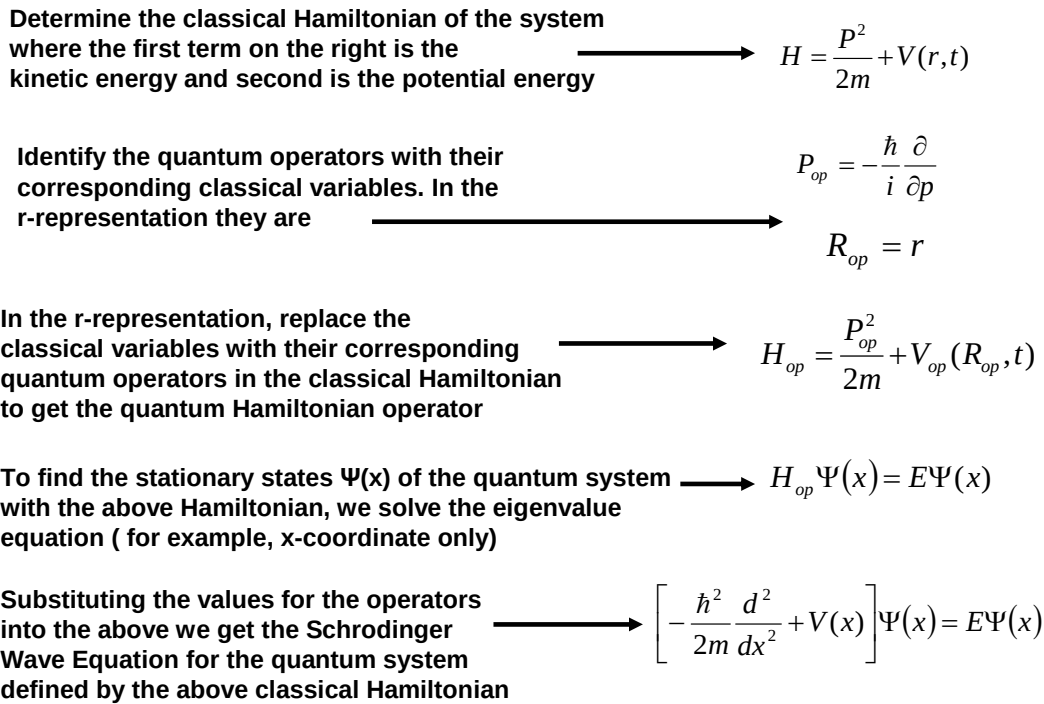


Figure 8.2 Determining the Schrodinger Wave Equation for a Quantum System

Using these quantum systems, the potential exists to develop nano-structures (i.e. quantum dots) that can confine a particle or system of particles whose state may be measured. The concept of a quantum bit (qubit) may be implemented, in one of its most simplest forms, as the intrinsic spin of an electron or as two states of the many states of a multistate system such as the geonium atom discussed in Chapter 6 or a simple quantum harmonic oscillator discussed in Chapter 5. Most of the work at present is focused on two state systems.

We showed two applications of the quantum computing paradigm. The Grover Search Algorithm was shown to provide $\sqrt{N}$ queries per search for a quantum approach as opposed to $N/2$ for a classical approach where N is the number of items in the database. An example was given for searching a linear image array for a specific pixel value. We also showed that the information contained by a qubit is almost twice that for a classical bit.

8.2 Discussion and Conclusion

In the past several years much effort has been put on the development of devices for building quantum computers. The Defense Advanced Research Projects Agency (DARPA) initiated a program about 5 years ago entitled Quantum Information Science and Technology (QuIST). The program objective is stated as follows:

The goal of the DARPA Quantum Information Science and Technolog (QuIST) program is to demonstrate advances required for practical use of quantum logic and information in computing, communications, and other applications. Specific areas of interest include:

1. fault-tolerant algorithms and architectures,
2. formulation of new algorithms and protocols for ultra-secure communications, ultra-precise metrology, information-bandwidth enhancements,
3. the limits of quantum computation for speedups over classical computation, and
4. computational applications for which quantum computation offers significant advantage over known classical equivalents.

Concurrently with these fundamental advances, QuIST seeks to develop the component technology for quantum computing and secure quantum communication including the development of robust megahertz rate single photon sources and detectors, practical implementations of single and multiple quantum bit logic gates, quantum memory, and systems level constructs such as quantum repeaters. The program is aimed at developing theory, hardware, and integrated demonstrations that may include scalable assemblies of quantum logic and memory, quantum teleportation-based communication, ultra-precise clock synchronization, communication of quantum information over large distances, and network backbones based on coherent optical and quantum techniques.

Under this program, the Massachusetts Institute of Technology (MIT), has proposed an architecture for a general purpose quantum computer²⁶. The architecture specifies a quantum memory, qubit refresh unit to aid in maintaining the state of a specific qubit, a quantum arithmetic logic unit (ALU), code teleporters, quantum wires, and a dynamic quantum compiler/scheduler which is a classical microprocessor. It also discusses the use of error correction since state decoherence noise is a problem in maintaining the state of the information. The architecture does not focus on any type of devices for constructing these components.

The area of quantum communications for secure communications appears to have a more near term maturity than quantum computing. There is even doubt among some that building a general purpose quantum computer may not be sufficiently competitive with present classical solid state computer technology. On the brighter side, special purpose quantum computers may be useful in providing exponential increases in compute power especially in the area of cryptography with possible use of Shor's algorithm^{27,25} for factorization.

8.3 Other research

In addition to the technology we presented in this report there is other work being conducted. This work includes Superconducting Quantum Interference Devices (SQUID)²⁸, Ion traps²⁹, Nuclear Magnetic Resonance (NMR), optical lattices³¹, and others. One only needs some imagination and a sound knowledge of quantum physics to devise a scheme to implement a qubit.

Glossary of Quantum Mechanics and Quantum Information Terms

Abelian Group – A group G is finite if the number of elements in G is finite. The order of a finite group G is the number of elements it contains. A group G is Abelian if $g_1 g_2 = g_2 g_1$ for all $g_1, g_2 \in G$. [Ref 2, pg. 610]

Action – product of energy and time

Annihilation operator – These operators are defined in terms of the position ($\mathbf{X}$) and momentum ($\mathbf{P}$) operators as follows: See also destruction operator. [Ref 2, pg. 284; Ref 5, pg. 489] for properties of these operators.

$$\mathbf{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega\mathbf{X} + i\mathbf{P})$$

BCS Theory – Named for John Bardeen, Leon Cooper, and Robert Schrieffer. According to theory, the electrons in a superconductor are coupled in pairs at low temperatures. The coupling comes about because of the interaction of electrons and the crystal lattice. At low temperatures ($T < T_C$), electron states called Cooper Pairs can be formed. T_C is the critical temperature below which superconductivity is experienced in a material. [Ref 21, p. 488].

Bijjective function – A function that is one to one and onto, i.e, for $f(x) = y$ there is precisely only one value of y .

http://www.wikipedia.com/wiki/Injective,_surjective_and_bijective_functions

Bloch Functions – Eigenfunctions of the wave equation for a periodic potential which are of the form of the product of a plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$ times a function $u_{\mathbf{k}}(\mathbf{r})$ with the periodicity of the crystal lattice. The solutions are composed of travelling waves, and they can be assembled into wave packets to represent electrons that propagate freely through the potential field of the ion cores. [Ref 10, p. 305 – 306].

Boltzman Distribution – Is given by $f_B(E) = 1/e^\alpha e^{E/kT}$ where E is the energy, k is the Boltzman constant, T is temperature and e^α is a system constant (sometimes denoted A). Note similarity between this and the Bose-Einstein and Fermi-Dirac Distributions. [Ref 21, p. 335].

Bohr magneton – It is closely equal to the spin magnetic moment of a free electron. This is a natural unit of measure for magnetic moment which has the value of $e\hbar / 2m_e = 9.27 \times 10^{-24}$ joules/Tesla = 5.79×10^{-5} eV/Tesla where m_e is the mass of the electron. [Ref 10, pg. 504].

Bohr Radius (a_0) – This is equal to $\hbar^2/mke^2 = 0.529$ Angstroms in the H atom for the smallest Bohr orbit possible for the electron in H ($n=1$). Bohr orbits for single electron atoms where $Z>1$ are closer to the nucleus than corresponding ones for the H atom. [Ref 21, p. 173].

Bosons – Particles which behave according to the Bose-Einstein Distribution. In a Bose-Einstein

gas there can be any number of particles in a single state. At very low temperatures there can be a significant number of particles in the ground state. Also particles with physical kets that are symmetric [$\psi(x_1, x_2) = \psi(x_2, x_1)$] are bosons. The constituents of most atoms are fermions but when assembled in such a way that the total spin of the ground state is integer (zero), the atoms are bosons in this lowest energy state. The x_1 and x_2 are space coordinates of two identical particles. [Ref 21, p. 350].

Bose-Einstein Condensation (BEC) – The process of molecules dropping into the ground state as their temperature is lowered below a critical temperature, T_c . The critical temperature for He atoms is about 3.1^0K . Also see BCS Theory. [Ref 21, p. 350].

Bose-Einstein Distribution - Given as $f_{BE}(E) = 1/(e^\alpha e^{E/kT} - 1)$ where E is energy, e^α is a system dependent normalization constant, T is temperature, k is the Boltzman constant. Bose realized that the Boltzman distribution did not adequately account for the behavior of photons so he created a new distribution for photons. Einstein generalized it to matter particles shortly thereafter giving this distribution. [Ref 21, p.350].

Bra – A bra symbolized by $\langle$ is defined to be a projection operator which projects a ket vector onto the unit vectors. Other definitions call a bra a “projector” and constructions like $\langle$ $\rangle$ projection operators. See Ket and Bracket.

Bracket – Is defined to be the action of a bra operator acting on a ket vector and symbolized as $\langle$ $\rangle$ and results in a projection operation of one vector onto another. Bra and Ket make a Bracket.

Collapse of Wavefunction – Using a vibrating string analogy, the collapse of the wavefunction means that a measurement of some observable such as energy or speed causes the wavefunction to suddenly collapse to one of the basis vectors. This is not true in the classical model for the vibrating string. One will observe just one vibrational mode (sine wave) after measurement although the string may have been vibrating in a more complex fashion before measurement.

Commutator - This is defined for two operators such that $[A, B] = AB - BA$. Not to be confused with the Poisson Bracket which involves partial derivatives of the two operators but is otherwise essentially the same. Hermitian Operators that commute represent observables that can be measured simultaneously.

Conservative System – Defined to have all of the forces derivable from a potential function. Also, such a system has constant total energy, i.e. the energy is conserved.

Cooper Pair – Charge carriers in superconductors have also been suggested as qubit representations. At low temperatures in certain metals, two electrons can bind together through phonon interaction to form a Cooper Pair, which has charge $2e$. And just as electrons can be confined with quantum dots, Cooper pairs can be confined with an electrostatic box, such that the number of cooper pairs in the box becomes a quantum number, and can be used to represent quantum information. Single qubit operations can be realized by using electrostatic gates to modulate the box potential, and Josephson junctions between coupled boxes. These junctions can also be used to couple qubits, and their strength can be modulated using an external magnetic

field by coupling appropriately to super-conducting interferometric loops. Finally, qubits can be measured simply by measuring electric charge. This superconductor qubit representation is interesting because of the relative robustness of Cooper pairs; it is estimated that the main decoherence mechanism is spontaneous emission of electromagnetic photons, which may allow coherence exceeding one microsecond, long compared with typical dynamical time scales of hundreds of picoseconds. (See BCS Theory). [Ref 2, p. 344]

deBroglie Wavelength - For a massive particle it is equal to h/mv where h is Planck's Constant, m = particle mass and v = particle velocity.

Density Operator - Alternate formulation for a quantum mechanical system. The density operator combines both quantum mechanics and statistical mechanics into one mathematical object. The quantum mechanical part of the density operator is related to the usual quantum mechanical wave function, which accounts for the inherent uncertainty for a particle. The statistical mechanics portion describes the lack of knowledge of the exact wave function for the particle or system because of macroscopic statistical processes. The operator is written as

$$\rho = \sum_{\Psi} P_{\Psi} |\Psi\rangle \langle \Psi|$$

Where P_{Ψ} represents an ensemble probability and describes our incomplete knowledge about macroscopic quantities and the system preparation and $|\Psi\rangle \langle \Psi|$ is related to the quantum mechanical probability which describes our lack of knowledge of microscopic quantities such as the location of an electron. It is the definition of the density operator above that most resembles the P-distribution of quantum optics.

Destruction operator – These operators are defined in terms of the position (**X**) and momentum (**P**) operators as follows:

$$a = \frac{1}{\sqrt{2m\hbar\omega}} (m\omega X - iP)$$

Diamagnetism - An effect caused by the changes in the orbital moment of a free atom induced by an applied magnetic field. Substances with a negative magnetic susceptibility are called diamagnetic. (See magnetic susceptibility)

Dual-Vector Space – The space dual to the vector space V is defined to be the set V^+ consisting of all of the bra operators. For each ket there is a bra and vice versa. Each element in the original vector space V is in 1-1 correspondence with the “dual vector space V^+ ”.

Ehrenfest's Theorem - This theorem shows how Schrodinger's quantum mechanics gives the usual results for classical mechanics. The time dependence of a wave function must be related to the time dependence of observed values.

Eigenstates - The eigenstates of a Hermitian operator, which corresponds to an observable, are

the most fundamental states for the particle or system. Every possible fundamental motion of a particle must be observable. This requires that each fundamental mode must be represented as a basis vector. The basis set must be complete to allow detection of the fundamental physical

modes. The basis set originates as the set of eigenvectors for the time-independent Schrodinger wave equation. The total wavefunction is made up of the basis set.

Electron Paramagnetic Resonance – [Ref 10, p. 604-606].

Electron Effective Mass - An electron in the conduction band of a crystal with a periodic potential due to lattice of atoms in the crystal is subject to forces not experienced in its free state. The Energy (E) versus wavevector (k) for the free electron is given as $E = \hbar^2 k^2 / 2m_e$ (see Section 5.1). If we compute the second order derivative with respect to k we get

$$\frac{1}{m_e} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}$$

However, electrons at the band edge of the conduction band experience a different E versus k curve so that the second derivative changes. Since $\hbar$ is constant, the mass of the electron has a different value according to the above equation. This value is called the effective mass (m^*) and is the value to be used in any dynamics that pertain to these band edge electrons. [Ref 21, p. 468-469]

Energy of a Particle – In wave mechanics the energy of a particle is given by $E = (\hbar/2\pi) \omega$ where ω is the angular frequency of the wavelike particle and $\hbar$ is Planck's constant.

Exciton – Bound electron-hole pair usually free to move together through a crystal. In some respects it is similar to an atom of positronium, which is formed from a positron and an electron. [Ref 10, p. 612].

Eulerian Angles – One can carry out the transformation from a given cartesian coordinate system to another by means of three successive rotations performed in a specific sequence. The Eulerian angles are then defined as the three successive angles of rotation. [Ref 6, p. 107].

Evolution Operator - This is given by $u(t) = \exp(\mathbf{H}/i\hbar)t$ and propagates the quantum mechanical wavefunction from $t=0$ to some time t. i.e. $\psi(t) = u(t) \psi(0)$

Fermions – Particles which obey the Fermi-Dirac Distribution. Also called Fermi-Dirac Particles. A gas containing Fermions can only have two particles in a single state. Also particles whose physical kets are antisymmetric [$\psi(x_1, x_2) = -\psi(x_2, x_1)$] are called fermions. The x_1 and x_2 are space coordinates of two identical particles. [Ref 21, p. 350].

Fermi-Dirac Distribution – Is given by $f_{FD}(E) = 1/(e^\alpha e^{E/kT} + 1)$ where E is energy, e^α is a system dependent normalization constant, T is temperature, k is the Boltzman constant. [Ref 21, p.350].

Fermi Energy – A system of fermions at $T=0$ is such that for $E < E_F$, $f_{FD}(E) = 1$ and for $E > E_F$, $f_{FD}(E) = 0$. Where f_{FD} is the Fermi-Dirac Distribution given above. One can write this distribution as $f_{FD}(E) = 1/(e^{(E-E_F)/kT} + 1)$. [Ref 21 p. 377].

Ferromagnetic Resonance – [Ref 10, p. 596 – 601].

also http://dpsg1.epfl.ch/cours/spin_dyn_final/ferromagnetic_resonance.htm

g-factor – This is called the spectroscopic splitting factor and is defined by $g \mu_B = -\gamma \hbar$ where μ_B is the Bohr Magnetron. It represents the ratio of the number of Bohr magnetons to the units of $\hbar$ of angular momentum. [Ref 10, pg. 504].

Gyromagnetic Ratio – In the expression for the magnetic moment $\mathbf{M} = \gamma \mathbf{J}$, γ is the gyromagnetic ratio, $\mathbf{M}$ is the magnetic moment and $\mathbf{J}$ is the angular momentum of a particle. For the electron the orbital gyromagnetic ratio is given by $\mu_B/h(\text{bar})$ and the spin gyromagnetic ratio is given as $2 \mu_B/h(\text{bar})$ where μ_B is the Bohr Magnetron. This is determined by the details of the charge distribution. In the case of the orbital angular momentum of the electron, $g=1$. [Ref 21, p. 308].

$\hbar$ – Planck's constant = $6.6 \times 10^{-34} \text{ kg}\cdot\text{m}^2\cdot\text{s}^{-1}$. (SI units).

$\hbar$ – $\hbar/2\pi$.

Hamiltonian – The Hamiltonian is the total energy of a system expressed in terms of the **generalized coordinates** $p, q, dp/dt, dq/dt$ and is equal to the sum of the total kinetic energy and potential energy where p =momentum, q = position.

Hermitian Operator – An operator O is Hermitian (self-adjoint) when $O^\dagger = O$. The term Hermitian is often reserved for complex Hilbert Spaces. Self adjoint operators have real eigenvalues and have orthogonal eigenvectors. All observables are represented by Hermitian operators.

Heisenberg Representation - The Heisenberg representation assigns dynamics to the operators. All of the wave functions, not just the basis set, are independent of time; none of the dynamics appears in the wave functions. The Schrodinger and Heisenberg representations of the Hamiltonian are physically identical.

Heisenberg Uncertainty – Elementary theory says that certain observables cannot be measured simultaneously with infinite precision. This is true for observables (operators) that do not commute. For example, the position and momentum operators do not commute, $\mathbf{P}\mathbf{x}\Psi \neq \mathbf{x}\mathbf{P}\Psi$ and the commutator is $[\mathbf{x}, \mathbf{P}] = i\hbar$. This is the uncertainty principle and can also be shown for other observables (operators) that do not commute.

Hilbert Space – A vector space with an inner product defined on it. Sometimes defined as a vector space of functions that are square integrable.

Interaction Representation - A hybrid between Schrodinger and Heisenberg Representations. Both operators and wave functions depend on time. The dynamics embedded in the wave function are due to the interaction. The operators carry the dynamics of the system that results when the interaction is turned off.

J – Total angular momentum of a system.

Ket - Denoted by $| \rangle$ and merely represents a vector . See Bra and Bracket

Lamb-Dicke Parameter /Criterion – This is a criterion which must be satisfied such that the width of the ion oscillation in the trap potential should be small compared to the wavelength of the incident light. It is expressed in terms of the Lamb-Dicke parameter $\eta \equiv 2\pi z_0/\lambda$ where λ is the wavelength, and $z_0 = \sqrt{\hbar / 2NM\omega}$ is the characteristic length scale of the spacing between ions in the trap. N is the number of ions in the trap, M is mass of each ion and ω is the angular frequency of the ion oscillation in the trap. [Ref 2, p. 312].

Larmor Frequency – The effect of a uniform magnetic field on a charged body with the torque $\mathbf{N} = \mathbf{M} \times \mathbf{B}$, where M is magnetic moment, is to cause the angular momentum vector to precess uniformly about $\mathbf{B}$ with an angular velocity $\omega_L = -e\mathbf{B}/2mc$ is known as the Larmor Frequency. (See Magnetic Moment (classical)).

Lowering Operator/Raising Operator – See Raising Operator.

Magnetization – The Magnetization $\mathbf{M}$ is defined as the magnetic moment per unit volume.

Magnetic Moment (classical) – The motion of charges as a result of the rotation of the body constitutes an electric current distribution which can interact with a magnetic field. If the field is uniform there will be no net force on the body but there will be a torque, approximately given by $\mathbf{N} = \mathbf{M} \times \mathbf{B}$ where $\mathbf{M}$ is the magnetic moment of the current distribution and $\mathbf{B}$ the magnetic intensity. For any volume distribution of current the magnetic moment is defined, in Gaussian units, $\mathbf{M} = 1/2c \int \mathbf{r} \times \mathbf{j} dV$ where $\mathbf{j}$ is the current density. The magnetic moment is related to the angular momentum $\mathbf{M} = (e/2mc)\mathbf{L}$. The magnetic moment of a free atom has three principal sources: (1) the spin with which electrons are endowed; (2) their orbital angular momentum about the nucleus; (3) and the change in the orbital momentum induced by an applied magnetic field. The **quantum magnetic moment** of an atom or ion is given as $\boldsymbol{\mu} = \gamma \hbar \mathbf{J} = -g\mu_B \mathbf{J}$. See Bohr magneton (μ_B), g-factor (g) and total angular momentum ($\mathbf{J}$). In the case of a charged particle with mass M and charge q moving in a current loop, the magnetic moment is the product of the current and the area of the loop. [Ref 21 p. 307].

Magnetic Susceptibility – The magnetic susceptibility per unit volume is given as $\chi = M/B$ where M is the magnetization and B is the macroscopic field intensity. (CGS units). [Ref 10, p. 499].

Magnons – The elementary excitations of a spin system have a wavelike form and are called **spin waves** or, when quantized are called **magnons**. These are analogous to lattice waves or phonons.

Meissner Effect - It has been observed experimentally that when a superconductor is cooled below its critical temperature in an external magnetic field, the magnetic field lines are expelled from the superconductor and thus the magnetic field inside the conductor is zero. The mechanism by which the magnetic lines are expelled or actually cancelled in the superconductor is that a supercurrent (called a screening current) is induced on the surface in such a direction as to exactly cancel the field within the material. [Ref 21, p. 485]

Momentum – In classical mechanics it is equal to mass times velocity (mv). In wave mechanics it is equal to the particle wavevector $\mathbf{k}$ times $\hbar$ ($\hbar/2\pi$).

Nuclear Magnetic Resonance – [Ref 10, p. 578-595].

Nuclear Quadrupole Resonance – This refers to observations of nuclear quadrupole splittings in the absence of a magnetic field. The quadrupole splitting is particularly large in covalently bonded molecules such as Cl_2 , Br_2 , and I_2 ; the splittings are of the order 10^7 or 10^8 Hz. Nuclei of spin $I \geq 1$ have an electric quadrupole moment. [Ref 10, p. 595- 596].

Observable – Each physical observable of a system corresponds to a Hermitian operator O_i , which induces a preferred basis set for the respective Hilbert space. The multiplicity of possible observables means that a single particle can “reside” in many Hilbert spaces at the same time since there can be a Hilbert space for each operator O_i (some operators might operate within the same space). The value of every physical observation must always be an eigenvalue of the Hermitian operator.

O(n) – The group of all real orthogonal $n \times n$ matrices. If we wish to restrict ourselves to those matrices with determinant +1 we speak of group $O^+(n)$. For example, $O(3)$ is the group of rotations in 3-D space; $O^+(3)$ is the group of *proper* rotations. [Ref 22, p. 450].

Paramagnetic – Atoms with a positive magnetic susceptibility

Pauli Exclusion Principle – No two electrons in an atom can have the same set of values for their four quantum numbers. Particles such as α -particles, deuterons, photons, and mesons have symmetric wave functions and do not obey the exclusion principle. A symmetric wave function is where $\psi(x_1, x_2) = \psi(x_2, x_1)$.

Phonon - The quantum of acoustic or vibrational energy, considered a discrete particle and used especially in mathematical models to calculate thermal and vibrational properties of solids.
<http://dictionary.reference.com/search?q=phonon>

Plasmon - A plasma oscillation in a metal is a collective longitudinal excitation of the conduction electron gas. A plasmon is a quantized plasma oscillation; we may excite a plasmon by passing an electron through a thin metallic film or by reflecting an electron (or a photon) from a film. [Ref 10, p. 276].

Polaron – An electron in a crystal lattice interacts via its electrical charge with the ions or atoms

of the lattice and creates a local deformation of the lattice. The deformation tends to follow the electron as it moves through the lattice. The combination of the electron and its strain field is known as a polaron. [Ref 10, p. 389].

Probability Density – This function measures the probability per unit length of per unit volume. In Quantum Theory, the probability density is given by $\rho = \Psi^* \Psi = |\Psi|^2$ such that Ψ must be normalized so that the integral of $|\Psi|^2$ over the volume is equal to 1.

Quantum Computing (Type II) - refers to a large parallel array of small quantum computers, connected together by classical communication channels. This is as opposed to the global coherence required in "Type I" quantum computers. For Grover's algorithm to work, however, an equal number of qubits must interact with each other as there are elements in the "database". Therefore, Type II QC will not work for Grover's algorithm in this regard. Shor's algorithm, which uses quantum Fourier transform, presumably will have the same problem. What Type II QC will enable is a very specific form of lattice-gas modeling. This is NOT a general purpose computer.

Quantum Dots – Quantum dots are fabricated semiconductor materials, metals, or even small molecules. They serve as 3-D boxes with electrostatic potentials which confine charge quanta. This is verified by observation of the Coulomb blockade effect, in which electrical conductance through dots of capacitance C is found to increase in discrete steps as a function of bias voltage across the dot, reflecting the $e^2/2C$ energy required to add each additional electron. Unlike photons, (net) charge cannot be destroyed; charges can only be moved around, and thus a charge state qubit would have to use something like the dual-rail representation, whereby the $|0\rangle$ and $|1\rangle$ states correspond to having charge located in either of two dots, or two states within a single dot.

Rabi Frequency/Oscillations – In a interaction between an atom-field system, the Rabi frequency is given by $\Omega = \sqrt{g^2 + \delta^2}$ where g represents the coupling constant between atom and field and δ is the detuning given by $\delta = (\omega_0 - \omega)/2$ where ω is the frequency of the field and ω_0 is the frequency of the atom. The atom and the field oscillate back and forth exchanging quantum of energy at the frequency Ω .

Raising Operator/Lowering Operator – The raising operator is defined as

$$\begin{aligned} L_+ &= L_x + iL_y \quad \text{raising operator} \\ L_- &= L_x - iL_y \quad \text{lowering operator} \end{aligned}$$

where L_x = component of angular momentum in the x direction
 L_y = component of angular momentum in the y direction

These operators enable us to represent all the eigenfunctions of L^2 and L_z using only one eigenfunction and the operators L_+ and L_- . $\mathbf{L}$ is the quantum mechanical angular momentum operator expressed in terms of the operators $\mathbf{r}$ and $\mathbf{p}$ such that $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. [Ref 23, p.98]

Raleigh Scattering – The process by which photons scatter elastically without a change in their frequency. In the classical theory, the oscillating electric field of the incident radiation produces

an oscillating acceleration of the atomic electrons, causing them to radiate at the same frequency as and in phase with the incident wave. Thus the electrons of the target atoms and molecules absorb energy from the incident wave and re-emit or scatter it in all directions without changing frequency. [Ref 21, p.416,414]

Raman Scattering – The incident and scattered photons are correlated in an inelastic scattering process. The scattered photon may have less energy than the incident photon or it may have greater energy if the molecule is initially in an excited vibrational or rotational energy state.

Thus, the scattered frequency is not the same as the incident frequency, nor is it related to a characteristic frequency of the molecule. It is found that for incident monochromatic radiation of frequency f the scattered radiation contains not only the frequency f (Raleigh scattering), but also much weaker lines on either side of the Raleigh line with frequencies given by $f' = f \pm \Delta f$. [Ref 21, p. 414, 417].

Schrodinger Representation - In this representation, the wavefunction is expressed as an expansion of energy eigenfunctions (no time dependence); they are stationary solutions of the time independent Schrodinger equation.(See Evolution Operator for dynamic solutions). The Schrodinger and Heisenberg representations of the Hamiltonian are identical.

Schrodinger Wave Equation – Is given as $\mathbf{H} \Psi = i \hbar \partial \Psi / \partial t$ where H is the classical Hamiltonian with the dynamical variables $\mathbf{p}$ (momentum) and $\mathbf{r}$ (position) are replaced by their respective operators, $\hbar$ is Plancks constant h divided by 2π and the derivative is a partial with respect to time.

Spin Waves – Oscillations in the relative orientations of spins on a lattice; lattice vibrations are oscillations in the relative positions of atoms in a lattice. [Ref 10, p.538].

Spin Wave Resonance – See Ferromagnetic Resonance.

Superconductivity – In some materials, there exists a temperature below which the resistivity is zero. These materials are called superconductors below this temperature. For example, Mercury is a superconductor below the critical temperature, T_c , or about 4^0K . Applying a magnetic field lowers the critical temperature. Recently, copper oxides have been found to have critical temperatures of up to 135^0K . [Ref 21, p.483]

Supercurrents – Currents that exist within a superconductor even when there is no electric field present. Currents have been observed for as long as years without any apparent loss in superconducting rings in which there is no field.

SU(n) – The group of all unimodular unitary $n \times n$ matrices, that is, the group of all $n \times n$ unitary matrices with determinant 1. It can be shown that $SU(n)$ has n^2-1 parameters. [Ref 22, p. 450].

Translation Operators - Translation and Rotation operators are unitary and have arguments that involve a Hermitian operator that is conjugate to the variable being rotated or translated.

Unitary Transformation - A “rotation” in the generalized Hilbert Space. A unitary operator has the property that $u^+ = u^{-1}$

Wavevector of Particle ($\mathbf{k}$) – is equal to $2\pi/\lambda$ where λ is the deBroglie wavelength of particle.

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